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Quantum Mechanics for Non-Hermitian Hamiltonians with PT Symmetries

Gustavo D. Duarte

Abstract

Quantum Mechanics is an axiomatic theory. One of its axioms states that every observable of a physical system is associated with a Hermitian operator allowing the reality of the energy spectrum and a complete set of eigenfunctions. Furthermore, because of the Hermicity imposed on the observable described by the Hamiltonian H, the time evolution of the system is preserved. In recent years, researchers have shown that the Hermicity requirement may be relaxed by a weaker condition described by the combined actions of $\mathcal{P}$ and $\mathcal{T}$ symmetries on the operator. Under this new regimen some non-Hermitian Hamiltonians have real spectra such as the complex extension of the harmonic oscillator. However, since the inner product of the $\mathcal{PT}$ symmetric Hamiltonian is not always positive definite a new inner product is defined with a new symmetry described by a $\mathcal{C}$ operator in order to construct a viable quantum mechanics theory.

In this thesis a succinct literature review of the $\mathcal{PT}$ symmetric non-Hermitian Hamiltonian theory is presented. The Hamiltonian $\mathcal{H} = p^2 + x^2(ix)^\varepsilon$ is discussed under $\mathcal{PT}$ transformation and its eigenvalues are calculated under numerical, asymptotic and semi-classical approximations. A two level Hamiltonian is introduced to showcase the main features of the $\mathcal{PT}$ symmetric theory. Moreover, the $\mathcal{CPT}$ inner product is constructed.

The objective of this thesis is to present to the reader a clear introduction of Quantum Mechanics for Non-Hermitian Hamiltonians with $\mathcal{PT}$ Symmetries where the principal concepts are explained step by step in order for the material to be accessible to the new reader.

MONTCLAIR STATE UNIVERSITY

Quantum Mechanics for Non-Hermitian Hamiltonians with $\mathcal{PT}$ Symmetries

by

Gustavo D. Duarte

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College of Science and Mathematics

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Thesis Committee:

Thesis sponsor: [redacted]

Dr. Ernest Ma

Committee Member: [redacted]

Dr. Aihua Li.

Committee Member: [redacted]

Dr. Bogdan Nita.

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1 Introduction

Classical Quantum Mechanics is a well recognized branch of physics. The model of the theory is based on a few postulates that generate the theoretical model. This model is based on two constructs: wave function and operators. The wave function is given by $\psi(x,t)$ and is obtained by solving the Schrödinger equation [19].

The description of physical observable quantities like position, momentum, energy, etc., are represented as Hermitian operators on the Hilbert space. A Hermitian operator is one that is linear and self-adjoint. A Hilbert space is a generalization of the Euclidean space which is a three-dimensional vector space provided with a dot product.[‡]

The Hamiltonian or energy of the system is represented by $H = T + V$, where T is the kinetic energy of the system and is constructed with the momentum operator $\hat{p}$ as follows

$$T = \frac{\hat{p}^2}{2m}, \tag{1.0.1}$$

where m is the mass of the system or particle and

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}. \tag{1.0.2}$$

In the same way V is the potential energy of the system and is constructed with the position operator $\hat{x}$, then

$$V = V(\hat{x}). \tag{1.0.3}$$

Then, the Hamiltonian of the system is given by

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}). \tag{1.0.4}$$

A classical quantum mechanical Hamiltonian must be Hermitian to describe a physical

[‡]See Appendix A.

system. A Hamiltonian is Hermitian if and only if it is invariant under simultaneous matrix-transposition and complex conjugation. This is represented symbolically by

$$H^{\dagger} = H, \tag{1.0.5}$$

where the symbol $(\dagger)$ denotes a Hermitian conjugate.

The Hermiticity imposed on the Hamiltonian is a sufficient condition for the reality of the energy spectrum, where the spectrum is defined as the collection of all the eigenvalues of an operator. Using the condition of Hermiticity on H and solving the time independent Schrödinger equation we obtain a real spectrum given by

$$\hat{H}\psi = E\psi, \tag{1.0.6}$$

where $\hat{H}$ is the Hamiltonian operator, ψ is the eigenfunction and E is the real eigenvalue [18]. Non-Hermitian Hamiltonians exist; however, these kinds of Hamiltonians are not part of the main cannon of classical quantum mechanics. Nonetheless, in recent years the condition of Hermiticity has been challenged as being too restrictive. In a pair of seminal papers, Bender and collaborators showed [5-6] using numerical, asymptotic and semi-classical techniques that the spectrum of $\mathcal{H}$ given below, which is not Hermitian[§] , includes real eigenvalues.

$$\mathcal{H} = p^2 + x^2(ix)^{\varepsilon}, \quad \varepsilon \in \mathbb{R}. \tag{1.0.7}$$

Furthermore, the eigenvalues of $\mathcal{H}$ are found to be real discrete and positive for $\varepsilon \geq 0$; in this case the energy levels increase as the parameter ε growths. If $-1 < \varepsilon < 0$ then we have a finite number of real eigenvalues and also an infinite number of complex conjugate pairs eigenvalues. As the parameter ε decreases from 0 to -1 the number of real eigenvalues decreases. Finally, as the parameter ε is less than -1 all the eigenvalues are complex [2].

[§]Proof given at Appendix B.

However, the last equation can be viewed as a complex extension of the harmonic oscillator Hamiltonian, which is included in the special case at $\varepsilon = 0$, where discrete energies are obtained as seen in Figure 1. Moreover, $\mathcal{H}$ possesses an anti-linear $\mathcal{PT}$ symmetry invariance under simultaneous space and $\mathcal{T}$ time reversal. Finally, it was proposed that the Hermiticity condition be replaced with the weaker requirement of space-time $\mathcal{PT}$ reflection invariance [15]. With this new condition, classical quantum mechanics can be extended in some cases into quantum mechanics for non-Hermitian Hamiltonians with $\mathcal{PT}$ symmetries.

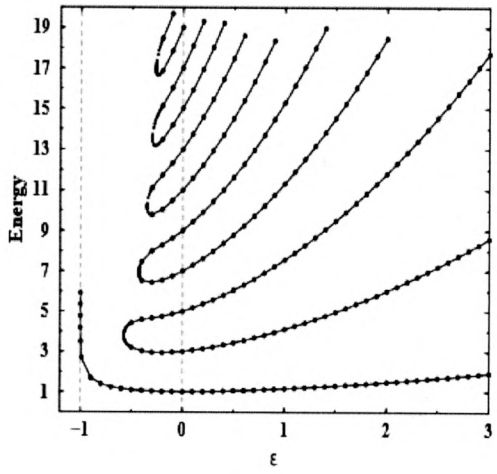

Figure 1: Eigenvalues of equation (1.0.7). We observe on the x axis the result of the different values of ε and on the y axis the values of energy given in units of $\frac{\hbar w}{2}$, where $\hbar$ is the Plank constant divided by 2π and w is the angular frequency. Notice that when ε is equal to zero we have the energy values of the quantum harmonic oscillator given by $(2n+1)$ where $n = (0, 1, 2, ...)$. We observe that when the parameter $\varepsilon > 0$ the eigenvalues are real discrete and positive. As the parameter ε changes from 0 to -1 the eigenvalues are both real and complex. If the parameter $\varepsilon < -1$ then we have complex eigenvalues [2].

This thesis will be organized as follows: In Chapter 2 we will describe the properties of $\mathcal{P}$ and $\mathcal{T}$ symmetries. In order to do so we will show examples of $\mathcal{P}$ and $\mathcal{T}$ acting alone and together on a system. Then, we will define the basics of $\mathcal{PT}$ quantum mechanics. In Chapter 3 we will apply the basics of the $\mathcal{PT}$ quantum mechanics theory to a two-level Hamiltonian system. In Chapter 4 we will discuss how to find the eigenvalues of $\mathcal{H}$ using WKB approximation, the name is an initialism for Wentzel-Kramers-Brillouin, semi-classical techniques and numerical approximations. We will discuss the spectrum of $\mathcal{H}$ in

the complex plane and do a case study for the following Hamiltonians

- $\mathcal{H} = p^2 + x^2(ix)^\varepsilon$,
- $\mathcal{H} = p^2 + ix^3$,
- $\mathcal{H} = p^2 + x^4$.

Finally, the last Chapter gives the conclusion of the paper.

2 $\mathcal{PT}$ Symmetries and Quantum Mechanics

2.1 $\mathcal{P}$ Parity Operator

The parity operator or space inversion is a symmetric transformation. If we apply parity operator to the standard coordinate system, it changes the right hand system into a left hand system. The parity operator in three-dimensional spaces is given by the following transformation

$$\mathcal{P}: \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix},$$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix}.$$

A matrix representation of parity in a finite number of dimensions has a determinant equal to -1 since parity by definition is a reflection [26].

In quantum mechanics, the parity transformation $(\mathcal{P})$ is a linear and unitary operator[‡] that performs a spatial inversion which reverses the sign of the position operator $\hat{x}$.

$$\mathcal{P}x = -x, \tag{2.1.1}$$

$$\mathcal{P}\hat{x}\mathcal{P} = -\hat{x}, \tag{2.1.2}$$

where equation (2.1.1) is the active transformation and equation (2.1.2) is the passive transformation of parity [2, 28]. The active transformation is a change in the physical position of a point and the passive transformation is a change on the coordinate system where the

[‡]See Appendix A.

object is located. If we apply condition (2.1.1) to the wave function, we obtain

$$\mathcal{P}\psi(x) = \psi(-x).$$

Applying condition (2.1.2) to position states $|x\rangle$ where the label x in the ket is the value of the position, we have

$$\begin{aligned}
\mathcal{P}\hat{x}\mathcal{P}\,|x_0\rangle &= \mathcal{P}\hat{x}\,|-x_0\rangle \\
&= \mathcal{P}(-x_0)\,|-x_0\rangle \\
&= -x_0\mathcal{P}\,|-x_0\rangle \\
&= -\hat{x}\,|x_0\rangle \\
\mathcal{P}\hat{x}\mathcal{P} &= -\hat{x},
\end{aligned}$$

where the position operator acting on a position state is defined as $\hat{x}\,|x_0\rangle = x_0\,|x_0\rangle$.

Since $\mathcal{P}$ operator is unitary, then $\hat{x}$ and $\mathcal{P}$ must anticommute. The anticommute condition is given when the swapping of any two arguments negate the results. The $\mathcal{P}$ operator is defined as an involutory and Hermitian transformation; therefore, we have the following properties

$$\mathcal{P}^2 = 1, \tag{2.1.3}$$

$$\mathcal{P}^{-1} = \mathcal{P}^\dagger = \mathcal{P}. \tag{2.1.4}$$

Equation (2.1.3) implies that the eigenvalues of $\mathcal{P} = \pm 1$. In order to construct a matrix representation of $\mathcal{P}$ we define the matrix $\mathcal{P}_0$ as the diagonal matrix with the eigenvalues of $\mathcal{P}$ [12]. The matrix $\mathcal{P}_0$ of a two-dimensional case is given by

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Then, we define the most general parity matrix as follows

$$\mathcal{P} = \mathcal{R}\mathcal{P}_0\mathcal{R}^{-1}, \tag{2.1.5}$$

where $\mathcal{R}$ is an orthogonal matrix rotation.

In the specific case of a two-dimensional parity matrix we have the following

$$\mathcal{P} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} * \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} * \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}^{-1}$$

or

$$\mathcal{P} = \begin{pmatrix} \frac{\cos^2(\theta)}{\cos^2(\theta)+\sin^2(\theta)} - \frac{\sin^2(\theta)}{\cos^2(\theta)+\sin^2(\theta)} & \frac{2\cos(\theta)\sin(\theta)}{\cos^2(\theta)+\sin^2(\theta)} \\ \frac{2\cos(\theta)\sin(\theta)}{\cos^2(\theta)+\sin^2(\theta)} & \frac{\sin^2(\theta)}{\cos^2(\theta)+\sin^2(\theta)} - \frac{\cos^2(\theta)}{\cos^2(\theta)+\sin^2(\theta)} \end{pmatrix}.$$

Now, using the condition (2.1.4) we use the inverse of $\mathcal{P}$ to arrive at the most general two-dimensional parity matrix with one free parameter [5], which is given by

$$\mathcal{P} = \begin{pmatrix} \cos(2\theta) & \sin(2\theta) \\ \sin(2\theta) & -\cos(2\theta) \end{pmatrix}.$$

Notice that $\mathcal{P}$ matrix is symmetric[‡] and is a reflection since the determinant is -1. Moreover, if we use an angle of 45 degrees in the last matrix, which is a reflection given by $x = y$, then x exchanges its value with y. Therefore, the simplest representation of $\mathcal{P}$ in two dimensions is given by

$$\mathcal{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The parity operator $\mathcal{P}$ acting on the momentum operator $\hat{p}$ reverses the sign of $\hat{p}$. Also, the parity operator $\mathcal{P}$ and momentum operator $\hat{p}$ do not commute.

$$\mathcal{P}\hat{p} = -\hat{p}, \tag{2.1.6}$$

[‡]See Appendix A.

$$\mathcal{P}\hat{p}\mathcal{P} = -\hat{p}. \tag{2.1.7}$$

If we apply condition (2.1.6) to the momentum states $\hat{p}$, then we have

$$\begin{aligned}\mathcal{P}\left|p\right\rangle &= \int dx \mathcal{P}\left|x\right\rangle \left\langle x|p\right\rangle \\ &= \int dx \left|-x\right\rangle \left\langle x|p\right\rangle \\ &= \int dx \left|x\right\rangle \left\langle -x|p\right\rangle .\end{aligned}$$

But $\langle -x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}px} = \langle x| - p\rangle$, then

$$\begin{aligned}\mathcal{P}\left|p\right\rangle &= \int dx \left|x\right\rangle \left\langle x| - p\right\rangle \\ \mathcal{P}\left|p\right\rangle &= \left|-p\right\rangle .\end{aligned}$$

If we apply condition (2.1.7) to a wave function $\psi(x_0, t)$, then we have

$$\begin{aligned}\mathcal{P}\hat{p}\mathcal{P}\psi(x_0) &= \mathcal{P}\hat{p}\psi(-x_0, t) \\ &= \mathcal{P}[-i\hbar\tfrac{d}{dx}\psi(-x_0, t)] \\ &= \mathcal{P}(i\hbar\psi'(-x_0, t)) \\ &= (i\hbar\psi'(x_0, t)) \\ &= -\hat{p}\psi(x_0, t),\end{aligned}$$

where the momentum operator is defined by equation (1.0.2). Moreover, the commutation relation

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar, \tag{2.1.8}$$

is not changed by the $\mathcal{P}$ operator,

i.e. $$\begin{aligned}\mathcal{P}[\hat{x}, \hat{p}]\mathcal{P} &= \mathcal{P}[\hat{x}\hat{p} - \hat{p}\hat{x}]\mathcal{P} \\ &= (\mathcal{P}(\hat{x})\mathcal{P})(\mathcal{P}(\hat{p})\mathcal{P}) - (\mathcal{P}(\hat{p})\mathcal{P})(\mathcal{P}(\hat{x})\mathcal{P}) \\ &= (-\hat{x})(-\hat{p}) - (-\hat{p})(-\hat{x}) \\ &= \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar.\end{aligned}$$

As an example of parity operator consider the following complex Hamiltonian:

$$H_a = \begin{pmatrix} v_0 + i\gamma & k \\ k & v_0 - i\gamma \end{pmatrix},$$

where v_0, γ and k are real numbers. Then, the parity transformation of H_a is given by

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} * \begin{pmatrix} v_0 + i\gamma & k \\ k & v_0 - i\gamma \end{pmatrix} * \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} v_0 - i\gamma & k \\ k & v_0 + i\gamma \end{pmatrix}$$

or

$$\mathcal{P}H_a\mathcal{P} = \begin{pmatrix} v_0 - i\gamma & k \\ k & v_0 + i\gamma \end{pmatrix}.$$

Now consider the Hamiltonian $\mathcal{H}$ in equation (1.0.7) under parity:

$$\begin{aligned} \mathcal{P}\mathcal{H}\mathcal{P} &= \mathcal{P}[(p)^2 + (x)^2(ix)^\varepsilon]\mathcal{P} \\ &= (\mathcal{P}(p)\mathcal{P})(\mathcal{P}(p)\mathcal{P}) + (\mathcal{P}(x)\mathcal{P})(\mathcal{P}(x)\mathcal{P})(\mathcal{P}(ix)^\varepsilon\mathcal{P}) \\ &= (-p)(-p) + (-x)(-x)((i)(-x))^\varepsilon \\ &= (p)^2 - (x)^2(ix)^\varepsilon, \end{aligned}$$

and therefore, $\mathcal{H} \neq \mathcal{P}\mathcal{H}\mathcal{P}$.

2.2 $\mathcal{T}$ Time Reversal Operator

Time reversal in classical mechanics is a reflection defined as $x(t) = x(-t)$, then

$$x'(t) = \frac{dx}{dt}(-t) = -\frac{dx}{d(-t)}(-t) = -x'(-t), \tag{2.2.1}$$

$$x''(t) = \frac{dx'}{dt}(t) = -\frac{dx'}{dt}(-t) = \frac{dx'}{d(-t)}(-t) = x''(-t). \tag{2.2.2}$$

Then, under time reversal the velocity changes signs but the position and the acceleration

do not. The time reversal transformation $\mathcal{T}$ is an anti-unitary and anti-linear[‡] operator [16, 27]. In quantum mechanics, time reversal operator $\mathcal{T}$ performs a complex conjugation, which leaves the operator $\hat{x}$ invariant and changes the sign of $\hat{p}$ operator. Then we have the following equations

$$\mathcal{T}\hat{x}\mathcal{T} = \hat{x}, \tag{2.2.3}$$

$$\mathcal{T}\hat{p}\mathcal{T} = -\hat{p}, \tag{2.2.4}$$

$$\mathcal{T}i\mathcal{T} = -i. \tag{2.2.5}$$

If we apply condition (2.2.3) to the wave function $\psi(x_0, t)$, then we have

$$\begin{aligned}\mathcal{T}\hat{x}\mathcal{T}\psi(x_0,t) &= \mathcal{T}\hat{x}\psi^*(x_0,-t)\\ &= \mathcal{T}x_0\psi^*(x_0,-t)\\ &= x_0\psi(x_0,t)\\ &= \hat{x}\psi(x_0,t).\end{aligned}$$

If we apply condition (2.2.4) to the wave function $\psi(x_0, t)$, then we have

$$\begin{aligned}\mathcal{T}\hat{p}\mathcal{T}\psi(x_0,t) &= \mathcal{T}\hat{p}\psi^*(x_0,-t)\\ &= \mathcal{T}[-i\hbar\tfrac{d}{dx}\psi^*(x_0,-t)]\\ &= \mathcal{T}(-i\hbar(\psi^*)'(x_0,-t))\\ &= (i\hbar\psi'(x_0,t))\\ &= -\hat{p}\psi(x_0).\end{aligned}$$

In order to show the anti-linearity of the time reversal operator [15] we use the commutator relation (2.1.8), then

$$\begin{aligned}\mathcal{T}[\hat{x},\hat{p}]\mathcal{T} &= \mathcal{T}[\hat{x}\hat{p}-\hat{p}\hat{x}]\mathcal{T}\\ &= (\mathcal{T}(\hat{x})\mathcal{T})(\mathcal{T}(\hat{p})\mathcal{T}) - (\mathcal{T}(\hat{p})\mathcal{T})(\mathcal{T}(\hat{x})\mathcal{T})\end{aligned}$$

[‡]See Appendix A.

$$= (\hat{x})(-\hat{p}) - (-\hat{p})(\hat{x})$$
$$= -\hat{x}\hat{p} + \hat{p}\hat{x} = (-1)(\hat{x}\hat{p} - \hat{p}\hat{x}) = (-1)(i\hbar)$$
$$= -i\hbar.$$

This confirms the anti-linear property of $\mathcal{T}$. Then, if we apply condition (2.2.5) to the wave equation $\psi(x_0, t)$, we have

$$\mathcal{T}i\mathcal{T}\psi(x_0, t) = \mathcal{T}i\psi^*(x_0, -t)$$
$$= \mathcal{T}[i\psi^*(x_0, -t)]$$
$$= (-i\psi(x_0, t))$$
$$= -i\psi(x_0, t).$$

Another property of $\mathcal{T}$ is that the square of $\mathcal{T}$ equals the unit operator and the inverse of $\mathcal{T}$ is equal to $\mathcal{T}$.

$$\mathcal{T}^2 = 1, \tag{2.2.6}$$

$$\mathcal{T}^{-1} = \mathcal{T}. \tag{2.2.7}$$

Consider a generic transformation $\mathcal{T}$ as follows

$$\mathcal{T} = \begin{pmatrix} \mathcal{T}_c & 0 \\ 0 & \mathcal{T}_c \end{pmatrix},$$

where $\mathcal{T}_c x = x^*$ and x^* is the complex conjugate of x. Then, the Hamiltonian H_a under time reversal operator is as follows

$$\begin{pmatrix} \mathcal{T}_c & 0 \\ 0 & \mathcal{T}_c \end{pmatrix} * \begin{pmatrix} v_0 + i\gamma & k \\ k & v_0 - i\gamma \end{pmatrix} = \begin{pmatrix} v_0 - i\gamma & k \\ k & v_0 + i\gamma \end{pmatrix}$$

or

$$\mathcal{T}H_a = \begin{pmatrix} v_0 - i\gamma & k \\ k & v_0 + i\gamma \end{pmatrix}.$$

Now let's consider the Hamiltonian $\mathcal{H}$ on equation (1.0.7) under time reversal $\mathcal{T}$:

$$\begin{aligned}
\mathcal{T}\mathcal{H}\mathcal{T} &= \mathcal{T}[(p)^2 + x^2(i)x^{\varepsilon}]\mathcal{T} \\
&= (\mathcal{T}(p)\mathcal{T})(\mathcal{T}(p)\mathcal{T}) + (\mathcal{T}(x)\mathcal{T})(\mathcal{T}(x)\mathcal{T})(\mathcal{T}(ix)^{\varepsilon}\mathcal{T}) \\
&= (-p)(-p) + (x)(x)((-i)(x))^{\varepsilon} \\
&= (p)^2 + (x)^2(-ix)^{\varepsilon}.
\end{aligned}$$

Therefore, $\mathcal{H} \neq \mathcal{T}\mathcal{H}\mathcal{T}$.

2.3 $\mathcal{PT}$ Symmetric System

We define a $\mathcal{PT}$ symmetric Hamiltonian to be one that satisfies the space-time reflection symmetry as follows.

Definition 1. *If*

$$H = H^{\mathcal{PT}}, \tag{2.3.1}$$

where

$$H^{\mathcal{PT}} \equiv (\mathcal{PT})H(\mathcal{PT}), \tag{2.3.2}$$

then H is called $\mathcal{PT}$ symmetric.

The matrix representation of H is symmetric with respect to the main diagonal [20]. Notice that the operators $\mathcal{P}$ and $\mathcal{T}$ commute, which is given by

$$[\mathcal{P}, \mathcal{T}] = \mathcal{PT} - \mathcal{TP} = 0. \tag{2.3.3}$$

Lemma 1. *If the Hamiltonian is $\mathcal{PT}$ symmetric, then the Hamiltonian commutes with the combined $\mathcal{PT}$ operator i.e. $[H, \mathcal{PT}] = 0$ or $\mathcal{P}H = H^*\mathcal{P}$.*

Proof. We want to prove that $[H, \mathcal{PT}] = 0$ *or* $\mathcal{P}H = H^*\mathcal{P}$.

Given: H is $\mathcal{PT}$ symmetric. The operators $\mathcal{P}$ and $\mathcal{T}$ commute. The Hamiltonian under time reversal operator is equal to the transpose conjugate of the Hamiltonian, $H^* = \mathcal{T}H\mathcal{T}$. The inverse of the parity operator is equal to the parity operator, $\mathcal{P}^{-1} = \mathcal{P}$. The parity operator square is equal to 1, $\mathcal{P}^2 = 1$. The parity operator times its inverse is equal to one, $\mathcal{P}\mathcal{P}^{-1} = 1$. The time reversal operator square is equal to 1, $\mathcal{T}^2 = 1$. The inverse of the time reversal operator is equal to the time reversal operator, $\mathcal{T}^{-1} = \mathcal{T}$. The time reversal operator times its inverse is equal to one, $\mathcal{T}\mathcal{T}^{-1} = 1$.

Begin proof: if $(\mathcal{PT})H(\mathcal{PT}) = H$

$\Rightarrow \mathcal{PT}H\mathcal{TP} = H$

$\Rightarrow \mathcal{PT}H\mathcal{T}(\mathcal{P}\mathcal{P}^{-1}) = H\mathcal{P}^{-1}$

$\Rightarrow \mathcal{PT}H\mathcal{T} = H\mathcal{P}$

$\Rightarrow \mathcal{PT}H(\mathcal{T}\mathcal{T}^{-1}) = H\mathcal{PT}^{-1}$

$\Rightarrow \mathcal{PT}H = H\mathcal{PT}.$

Therefore, $[H, \mathcal{PT}] = 0$.

Second, if H and $\mathcal{PT}$ commute, then

$H\mathcal{PT} = \mathcal{PT}H$

$\Rightarrow H\mathcal{TP} = \mathcal{TP}H$

$\Rightarrow \mathcal{T}^{-1}H\mathcal{TP} = (\mathcal{T}^{-1}\mathcal{T})\mathcal{P}H$

$\Rightarrow (\mathcal{T}H\mathcal{T})\mathcal{P} = \mathcal{P}H$

$\Rightarrow H^*\mathcal{P} = \mathcal{P}H.$

Therefore, we have proved that $[H, \mathcal{PT}] = 0$ or $\mathcal{P}H = H^*\mathcal{P}$, as required.

□

Despite the fact that $\mathcal{PT}$ Hamiltonians can, in general be non-Hermitian, their spectra can be entirely real. Such systems, since they commute, share the same eigenfunctions

between the Hamiltonian H and the $\mathcal{PT}$ operator [2].

Suppose

$$\mathcal{PT}\psi = \lambda\psi, \tag{2.3.4}$$

where λ is equal to E and represents the eigenvalues of the equation.

Multiply the last equation by $\mathcal{PT}$ from the left. Then we have

$$(\mathcal{PT})(\mathcal{PT})\psi = (\mathcal{PT})\lambda\psi$$

$$\Rightarrow \psi = (\mathcal{PT})\lambda(\mathcal{PT})^2\psi$$

$$\Rightarrow \psi = [(\mathcal{PT})\lambda(\mathcal{PT})](\mathcal{PT})\psi,$$

since

$$(\mathcal{PT})^2 = 1. \tag{2.3.5}$$

Then,

$$\psi = \lambda^*\lambda\psi = |\lambda|^2\psi. \tag{2.3.6}$$

Therefore, $|\lambda|^2 = 1$ and the eigenvalue λ of the $\mathcal{PT}$ operator has a norm of one

$$|\lambda| = 1. \tag{2.3.7}$$

Therefore,

$$\lambda = e^{i\alpha}. \tag{2.3.8}$$

Then, the eigenvalue is a phase factor and is part of the circle group which is the multiplicative group of complex numbers with absolute value equal to one. However, if we generalize condition (2.3.4), then

$$\mathcal{PT}\psi_n(x) = \lambda_n\psi_n(x), \tag{2.3.9}$$

$$|\lambda_n| = 1 \rightarrow \lambda_n = e^{(i\alpha)_n}. \tag{2.3.10}$$

If the n phase is absorbed into the eigenfunction and rescaled, then we have the normalized eigenfunction

$$\psi_n(x) \rightarrow e^{(\frac{i\alpha_n}{2})}\psi_n(x). \tag{2.3.11}$$

The last normalization satisfies the following condition

$$\mathcal{PT}\psi_n(x) = \psi_n^*(-x) = \psi_n(x). \tag{2.3.12}$$

In general, the spectrum of a $\mathcal{PT}$ symmetric Hamiltonian shows a broken symmetric phase; we define the broken phase where the spectrum becomes partially or completely complex. If the phase is broken, some of the eigenfunctions of $H^{\mathcal{PT}}$ are not simultaneously eigenfunctions of the $\mathcal{PT}$ operator. The unbroken phase is where both H and $\mathcal{PT}$ share the same set of eigenfunctions. This corresponds to the so-called exact $\mathcal{PT}$-symmetric phase and in this case the spectrum is real.

Moreover, multiply the eigenvalue problem (1.0.6) by $(\mathcal{PT})$ from the left side and we have

$(\mathcal{PT})H\psi = (\mathcal{PT})E\psi$

$\Rightarrow H(\mathcal{PT})\psi = (\mathcal{PT})E\psi$

$\Rightarrow H\lambda\psi = (\mathcal{PT})E(\mathcal{PT})^2\psi$

$\Rightarrow H\lambda\psi = [(\mathcal{PT})E(\mathcal{PT})](\mathcal{PT})\psi$

$\Rightarrow H\lambda\psi = E^*\lambda\psi$

$\Rightarrow E\lambda\psi = E^*\lambda\psi.$

Therefore, $E\psi = E^*\psi$.

The last equation states that the eigenvalues are real but this condition is only true on the unbroken phase of the $H^{\mathcal{PT}}$ system. For the specific case of the Hamiltonian (1.0.7)

the condition is true if $\varepsilon \geq 0$, in which case the system shows an unbroken phase but if $\varepsilon < 0$ then the system presents a broken phase. Now, let's consider $\mathcal{H}$ under parity and time transformation as follows

$$\begin{aligned}\mathcal{PT}\mathcal{H}\mathcal{PT} &= \mathcal{PT}[p^2 + (x)^2(ix)^\varepsilon]\mathcal{PT} \\ &= (\mathcal{PT}(p)\mathcal{PT})(\mathcal{PT}(p)\mathcal{PT}) + (\mathcal{PT}(x)\mathcal{PT})(\mathcal{PT}(x)\mathcal{PT})((\mathcal{PT}(ix)^\varepsilon\mathcal{PT})) \\ &= (p)(p) + (-x)(-x)((-i)(-x))^\varepsilon \\ &= (p)^2 + (x)^2(ix)^\varepsilon.\end{aligned}$$

Therefore, $\mathcal{H} = \mathcal{PT}\mathcal{H}\mathcal{PT}$.

2.4 Pseudo-Hermiticity

The condition of Hermiticity in a quantum mechanical system can be replaced for a more relaxed condition of a $\mathcal{PT}$ symmetric system. In turn a $\mathcal{PT}$ symmetric system belongs to a more general mathematical context known as pseudo-Hermiticity. We will use this concept to define a more general $\mathcal{PT}$ symmetric Hamiltonian in this section.

Definition : A linear operator $A : \mathcal{H} \to \mathcal{H}$ acting on a separable Hilbert space $\mathcal{H}$ is said to be pseudo-Hermitian if $\mathcal{D}(A)$ is a dense subset of $\mathcal{H}$, and there is an everywhere defined invertible Hermitian linear operator $\eta : \mathcal{H} \to \mathcal{H}$ such that

$$A^\dagger = \eta A \eta^{-1}. \tag{2.4.1}$$

A Hilbert space is separable if it has a countable orthonormal basis; a separable Hilbert space is isometric or congruent to L^2, the space of square integrable functions.[‡] Dense is defined as follows: "E is dense in X if every point of X is a limit point of E or a point of E or both, where X is a metric space" [25].

Condition (2.4.1) reduces the ordinary Hermiticity if $\eta = 1$, then η is the identity operator. If the η operator is given by $\mathcal{P}$ which is Hermitian and A is replaced by H in the same equation, then it follows that H is Pseudo-Hermitian [22]. This means

[‡]See Appendix A.

$$H^{\dagger} = \mathcal{P}H\mathcal{P} \tag{2.4.2}$$

and

$$H = \mathcal{P}H^{\dagger}\mathcal{P}, \tag{2.4.3}$$

where $H^{\dagger}$ is the transpose conjugate of H. The last equation is the most general definition of a Hamiltonian under parity and time reflection since

$$\begin{aligned} & H = \mathcal{P}H^{\dagger}\mathcal{P} \\ \Rightarrow\ & H = \mathcal{P}(\mathcal{T}H\mathcal{T}^{-1})\mathcal{P} \\ \Rightarrow\ & H = (\mathcal{P}\mathcal{T})H(\mathcal{T}\mathcal{P}) \\ \Rightarrow\ & H = (\mathcal{P}\mathcal{T})H(\mathcal{P}\mathcal{T}), \end{aligned}$$

where we recover the definition (2.3.2) of $\mathcal{PT}$ symmetric Hamiltonian.

The simplest physical model showing $\mathcal{PT}$ symmetric properties is the two-level system [31]. Consider once again the Hamiltonian H_a. Clearly this Hamiltonian is non-Hermitian since $H_a \neq H_a^{\dagger}$:

$$\begin{pmatrix} v_0 + i\gamma & k \\ k & v_0 - i\gamma \end{pmatrix} \neq \begin{pmatrix} v_0 - i\gamma & k \\ k & v_0 + i\gamma \end{pmatrix}.$$

Moreover, H_a is a two-level system with a coupling parameter k, where v_0, γ and k are real numbers. This Hamiltonian is $\mathcal{PT}$ symmetric since it follows the condition (2.4.3), then

$$\begin{pmatrix} v_0 + i\gamma & k \\ k & v_0 - i\gamma \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} * \begin{pmatrix} v_0 - i\gamma & k \\ k & v_0 + i\gamma \end{pmatrix} * \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The eigenvalues of the Hamiltonian H_a can be found via diagonalization[§] to be

[§]See Appendix B for exact calculations.

$$E_{\pm} = v_0 \pm \sqrt{k^2 - \gamma^2}, \tag{2.4.4}$$

which represent the two energy eigenvalues [3]. From the eigenvalues equation we observe that when $\gamma^2 < k^2$, the energy eigenvalues are real and the phase is unbroken. When $\gamma^2 > k^2$, the energy eigenvalues are complex and the phase of the system is broken. The transition from a real to a complex spectrum takes place at $\gamma = y = 1$ and -1. These two points are where the phase changes from unbroken to broken as can be seen in Figure 2.

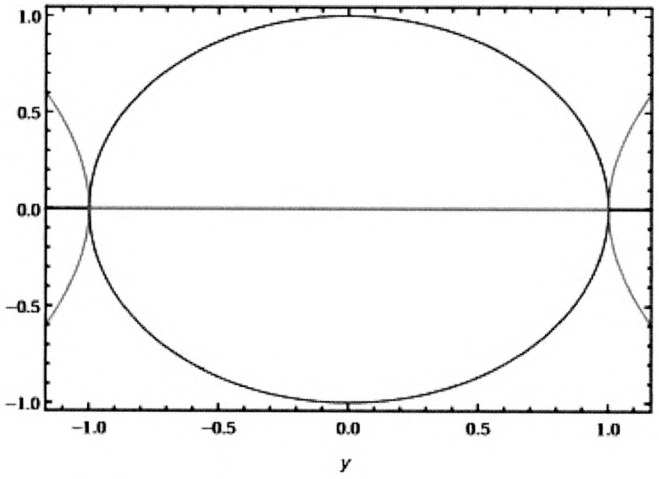

Figure 2: Eigenvalues of the simple $\mathcal{PT}$ symmetric system described by the matrix model H_a. In order to obtain the exact graph $v_0 \to 0$ and $k = \gamma = 1$. We observe on the graph unbroken symmetry between 1 and -1, otherwise the symmetry is broken and we have complex eigenvalues. Figure 2 was obtained by using Wolfram Alpha online program.

2.5 $\mathcal{PT}$ Quantum Mechanics

In this section we will compare classical quantum mechanics against non-Hermitian quantum mechanics. We will use the postulates of classical quantum mechanics and express the same postulates in non-Hermitian quantum mechanics whenever possible.

The formalism of the classical quantum mechanics theory [18-19] can be described as follows:

- The description of the system postulates that the wave function describes a quantum

mechanical system through its spatial and time dependence. The state of a quantum mechanical system is completely specified by the wave function $\psi(x,t)$, which belongs inside an abstract space known as the Hilbert space.

The Hilbert space is provided with a dot product or inner product. We define this inner product between two functions $f(x)$ and $g(x)$ as follows

$$\langle f|g\rangle \equiv \int_a^b f(x)^* g(x) dx. \tag{2.5.1}$$

If $f(x)$ and $g(x)$ are both square integrable[‡], the inner product exists and converges to a finite number.

The equation (2.5.1) satisfies all the conditions of the inner product. In particular we observed that

$$\langle g|f\rangle = \langle f|g\rangle^* . \tag{2.5.2}$$

Meanwhile, the inner product of $f(x)$ with itself, is defined as

$$\langle f|f\rangle = \int_a^b |f(x)|^2 dx, \tag{2.5.3}$$

which is real and non-negative and it is zero only when $f(x) = 0$. A function is normalized if the inner product with itself is equal to 1. A pair of functions is orthogonal if their inner product is 0. A set of functions are orthonormal if they are normalized and orthogonal. Then,

$$\langle f_m|f_n\rangle = \delta_{mn}, \tag{2.5.4}$$

where δ_{mn} is the Kronecker delta function of two variables defined as

[‡]See Appendix A.

$$\delta_{mn} = \begin{cases} 0 \ if \ \ m \neq n \\ 1 \ if \ \ m = n. \end{cases} \tag{2.5.5}$$

A set of functions is complete if any function in the Hilbert space can be expressed as a linear combination of them

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x), \tag{2.5.6}$$

where if the function is orthonormal then c_n is given by

$$c_n = \langle f_n | f \rangle . \tag{2.5.7}$$

Notice that condition (2.5.6) can be expressed as

$$|\psi\rangle = \sum_n c_n \, |\phi_n\rangle , \tag{2.5.8}$$

$$\sum_n \langle \phi_n | \psi \rangle \, |\phi_n\rangle = \left(\sum_n |\phi_n\rangle \, \langle \phi_n| \right) |\psi\rangle , \tag{2.5.9}$$

which implies that

$$\sum_n |\phi_n\rangle \, \langle \phi_n| = 1. \tag{2.5.10}$$

Using the delta function the completeness statement in a space coordinate is the reconstruction of the unit operator as a sum over the eigenfunctions, then

$$\sum_{n=1}^{\infty} [\psi_n(x)]^* \psi_n(y) = \delta(x - y). \tag{2.5.11}$$

In non-Hermitian quantum mechanics the states of the system are also completely specified by its wave function. However, in general, the eigenfuction of non-Hermitian operators are not orthogonal with respect to this inner product.

The inner product between two eigenfunctions of a $\mathcal{PT}$ system is defined as

$$(\psi, \phi) = \int_C \psi(x)^{\mathcal{PT}} \phi(x) dx = \int_C \psi(-x)^* \phi(x) dx, \tag{2.5.12}$$

where C is the contour defined in the region on the complex plane, where the Schrödinger equation can be solved using WKB theory,[‡‡] also known as Stokes wedges [5].

With this definition of the inner product, two eigenfunctions are orthogonal; however, this definition fails to produce a positive norm [29].

Thus,

$$\int_C \psi_n(x)^{\mathcal{PT}} \psi_m(x) dx = \int_C \psi_n(-x)^* \psi_m(x) dx = 0. \tag{2.5.13}$$

Consider the following inner product where

$$\phi \rightarrow \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix},$$

$$(\phi^{\mathcal{PT}}, \phi) \Rightarrow \begin{pmatrix} \phi_1^* & \phi_2^* \end{pmatrix} * \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} * \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} \phi_1^* & \phi_2^* \end{pmatrix} * \begin{pmatrix} \phi_1 \\ -\phi_2 \end{pmatrix}$$

$$\Rightarrow \phi_1^* \phi_1 - \phi_2^* \phi_2 = |\phi_1|^2 - |\phi_2|^2.$$

[‡‡]WKB See Section 4.1. Wedges See Section 4.2.

The last equation is negative if $|\phi_2|^2 > |\phi_1|^2$. Moreover, using the $\mathcal{PT}$ definition (2.5.12) with eigenfunctions of the Hamiltonian given by equation (1.0.7) the resulting norm is $(-1)^n$ for all n and $\varepsilon > 0$ [8], then

$$\int_C \psi_n(x)^{\mathcal{PT}} \psi_n(x) dx = \int_C \psi_n(-x)^* \psi_n(x) dx = (-1)^n. \tag{2.5.14}$$

In order to enforce positive norm for non-Hermitian Hamiltonians having unbroken $\mathcal{PT}$ symmetry, the operator $\mathcal{C}$ is introduced to account for the negative values of the norm. The $\mathcal{C}$ operator is linear and commutes with both H and $\mathcal{PT}$. The $\mathcal{C}$ operator is a symmetry of H. The $\mathcal{C}$ operator takes its name from the charge conjugation operator in particle physics because of the similarities of the operations [20]. The $\mathcal{C}$ operator can be expressed in coordinate space as a sum over the $\mathcal{PT}$ normalized eigenstates of the $\mathcal{PT}$ symmetric Hamiltonian as follows:

$$\mathcal{C}(x, y) = \sum_{n=0}^{\infty} \phi_n(x) \phi_n(y). \tag{2.5.15}$$

One of the properties of the $\mathcal{C}$ operators is as follows

$$\mathcal{C}^2 = 1. \tag{2.5.16}$$

Then,

$$\int dy \mathcal{C}(x, y) \mathcal{C}(y, z) = \delta(x - z), \tag{2.5.17}$$

where δ is the delta function. Therefore, the eigenvalues of $\mathcal{C}$ are ± 1. Using the fact that $\mathcal{C}$ is linear and commutes with H, the eigenstates of H have definite values of $\mathcal{C}$, then

$$\mathcal{C}\phi_n(x) = \int dy \mathcal{C}(x, y) \phi_n(-y), \tag{2.5.18}$$

$$= \sum_{m=0}^{\infty} \phi_m(x) \int dy \phi_m(y)\phi_n(y) = (-1)^n \phi_n(x). \tag{2.5.19}$$

Using the $\mathcal{C}$ operator we define the new $\mathcal{CPT}$ inner product as follows:

$$\langle \psi, \phi \rangle^{\mathcal{CPT}} \equiv \int_C \psi(x)^{\mathcal{CPT}} \phi(x) dx, \tag{2.5.20}$$

where

$$\psi(x)^{\mathcal{CPT}} = \int \mathcal{C}(x,y)\psi^*(-y)dy. \tag{2.5.21}$$

Using this definition of the $\mathcal{CPT}$ inner product, two eigenfunctions are orthogonal and positive definitive. The completeness of the eigenfunction is defined as

$$\sum_{n=0}^{\infty} (-1)^n \phi_n(x)\phi_n(y) = \delta(x-y). \tag{2.5.22}$$

And in terms of the $\mathcal{CPT}$ inner product completeness is as follows

$$\sum_{n=0}^{\infty} \phi_n(x)[\mathcal{CPT}\phi_n(y)] = \delta(x-y). \tag{2.5.23}$$

- Observables and physical quantities are represented by Hermitian operators on the Hilbert space. This condition guarantees the reality of the expectation value of A, where A is an operator. However, in the Heisenberg picture, operators evolve with time and the Hermiticity condition is maintained, then

$$A(t) = e^{iHt} A(0) e^{-iHt}. \tag{2.5.24}$$

A similar condition as in the Heisenberg picture is given for a $\mathcal{PT}$ symmetric system at $t = 0$, the operator A must obey the condition

$$A^T = \mathcal{CPT}A\mathcal{CPT}, \tag{2.5.25}$$

where A^T is the transposed operation of A. If the condition holds at $t = 0$, then it will hold at any other time for the Hamiltonian H because H is symmetric.[‡] This guarantees the expectation value of A is real.

Since the operator $\mathcal{C}$ satisfies the last requirement, then the operator $\mathcal{C}$ is an observable. The Hamiltonian is also an operator. But $\hat{x}$ and $\hat{p}$ are not. Thus, there is no position operator in a $\mathcal{PT}$ symmetric system.

- The temporal evolution of a quantum state is given as

$$\psi_t(x) = e^{-iHt}\psi_0(x). \tag{2.5.26}$$

In order to ensure that the norm remains unchanged with time, the temporal evolution must be unitary. The unitary evolution remains valid for $\mathcal{PT}$ symmetric Hamiltonians as long as the Hamiltonian commutes with the $\mathcal{CPT}$ operator within the inner product.

- The following postulates are the same in both theoretical models.

- The expansion postulate assumes that any wave function $\psi(x,t)$ of a quantum mechanics system can be expressed as a coherent superposition of a complete set.

- The measurement postulate states that for a single measurement of an observable corresponding to a quantum mechanical operator, only the eigenvalues of the operator will be measured.

- The reduction postulate in place guarantees the reproducibility of measurements, where a coherent superposition reduces to an eigenfunction upon measurement [19].

[‡]See Appendix A.

Finally, on the next table we present the main differences and similarities between classical quantum mechanics and non-Hermitian quantum mechanics.

Quantum Mechanics		
	Classical Quantum Mechanics	Non-Hermitian Quantum Mechanics
1-Hamiltonian.	Hermitian.	Non-Hermitian.
2-Schrodinger eigenvalue problem.	Solutions $\in \mathbb{R}$.	Solutions $\in \mathbb{R}, \mathbb{C}$.
3-Symmetries.	$\mathcal{P}$ and $\mathcal{T}$.	$\mathcal{P}$, $\mathcal{T}$ and $\mathcal{C}$. $\mathcal{C}(x,y) = \sum_{n=0}^{\infty} \phi_n(x)\phi_n(y).$
4-Inner product.	$\langle \psi \vert \psi \rangle = \int \psi_m(x)^* \psi_n(x) dx.$	$\langle \psi, \phi \rangle^{\mathcal{CPT}} \equiv \int_C \psi(x)^{\mathcal{CPT}} \phi(x) dx.$
5-Unitary temporal evolution.	$\psi_t(x) = e^{-iHt}\psi_0(x).$	$\psi_t(x) = e^{-iHt}\psi_0(x).$
6-Observables.	$A = A^\dagger.$	$A^T = \mathcal{CPT}A\mathcal{CPT}.$

Table 1: Features of Classical Quantum Mechanics vs. non-Hermitian Quantum Mechanics.

3 Hamiltonian of a Two-Level System

In this section we expand on the Hamiltonian of a two-level system. Because of the simplicity of this system, we can show the most important features of the Hamiltonian with $\mathcal{PT}$ symmetry. The two-level system is constructed as follows. Suppose we have an isolated system with a (x, y, z) coordinate plane. We impose a source at a distance r from the center of x then, the source is located at $x = r$. The most common source is an antenna that radiates energy at a constant rate. In the next step, we impose a sink at a distance $x = -r$. The most common sink is an antenna that absorbs energy [3]. If we apply the $\mathcal{P}$ operator to the system, then we exchange the positions of the source and sink. If we apply the $\mathcal{T}$ operator, the source becomes a sink and the sink becomes a source making the system $\mathcal{PT}$ symmetric. If the system is isolated the source goes to zero and the sink goes to infinity. In this case we are under the presence of broken $\mathcal{PT}$ symmetry and the eigenvalues of the Hamiltonian are complex. If the source and sink are strongly coupled, then the system can reach equilibrium. In other words, we are under the presence of an unbroken $\mathcal{PT}$ symmetric system and the eigenvalues of the Hamiltonian are real [4].

The Hamiltonian that represents the sink is given by $H = re^{+i\theta}$, where $r > 0$ and $0 < \pi < \theta$. The source is represented by $H = re^{-i\theta}$. If we put the source and the sink together in one Hamiltonian with a coupling parameter k in order to have an unbroken $\mathcal{PT}$ symmetric system, then we have the following complex Hamiltonian matrix

$$H_b = \begin{pmatrix} re^{+(i\theta)} & k \\ k & re^{-(i\theta)} \end{pmatrix},$$

where r, θ and k are real parameters. Mathematically, H_b represents the two-level system and is a similar matrix to H_a where $re^{\pm(i\theta)} = r[\cos(\theta) \pm i\sin(\theta)] = r[v_0 \pm i\gamma]$ if $r = 1$, $\cos(\theta) = v_0$ and $\sin(\theta) = \gamma$, where we use the Euler formula

$$e^{+(i\theta)} = \cos(\theta) + i\sin(\theta) \quad and \quad e^{-(i\theta)} = \cos(\theta) - i\sin(\theta). \tag{3.0.1}$$

Now, we will show that this system has all the properties of a $\mathcal{PT}$ symmetric Hamiltonian. H_b is not Hermitian since it does not comply with equation (1.0.5), then we have $H_b \neq H_b^\dagger$:

$$\begin{pmatrix} re^{+(i\theta)} & k \\ k & re^{-(i\theta)} \end{pmatrix} \neq \begin{pmatrix} re^{-(i\theta)} & k \\ k & re^{+(i\theta)} \end{pmatrix}.$$

Let us consider the two-level system under the parity transformation where the operator $\mathcal{P}$ is given by the general $\mathcal{P}$ matrix. Then, $\mathcal{P}H_b\mathcal{P} = H_b'$ where H_b' represents the transformation of H as follows

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} * \begin{pmatrix} re^{+(i\theta)} & k \\ k & re^{-(i\theta)} \end{pmatrix} * \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} re^{-(i\theta)} & k \\ k & re^{+(i\theta)} \end{pmatrix}$$

or

$$\mathcal{P}H\mathcal{P} = \begin{pmatrix} re^{-(i\theta)} & k \\ k & re^{+(i\theta)} \end{pmatrix}.$$

Now, we consider the same two-level Hamiltonian system under time transformation $\mathcal{T}$ then, H_b under time reversal operator is given by $\mathcal{T}H_b = H_b'$ where H_b' represents the transformation of H_b as below

$$\begin{pmatrix} \mathcal{T}_c & 0 \\ 0 & \mathcal{T}_c \end{pmatrix} * \begin{pmatrix} re^{+(i\theta)} & k \\ k & re^{-(i\theta)} \end{pmatrix} = \begin{pmatrix} re^{-(i\theta)} & k \\ k & re^{+(i\theta)} \end{pmatrix}$$

or

$$\mathcal{T}H_b = \begin{pmatrix} re^{-(i\theta)} & k \\ k & re^{+(i\theta)} \end{pmatrix}.$$

Note that the matrix H_b' is not equal to the original matrix H_b of the two-level system and H_b under time transformation is equal to the transport conjugate of the matrix H_b.

Now consider the Hamiltonian H_b under combined $\mathcal{PT}$ symmetry where the most general form of a $\mathcal{PT}$ invariant Hamiltonian satisfies equation (2.4.3), then

$$\begin{pmatrix} re^{+(i\theta)} & k \\ k & re^{-(i\theta)} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} * \begin{pmatrix} re^{-(i\theta)} & k \\ k & re^{+(i\theta)} \end{pmatrix} * \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

3.1 Broken and Unbroken Symmetry

In the last section we observed that the two-level system Hamiltonian is $\mathcal{PT}$ symmetric. In order to determine if the system has broken or unbroken symmetry we need to find the eigenvalues using the following equation

$$Det(A - \lambda I) = 0, \tag{3.1.1}$$

where A is a square matrix, λ is the eigenvalue and I is the identity matrix. Then, using $A = H$ in equation (3.1.1) we have the following $Det(H - \lambda I) = 0$, and solving the last equation we have the following eigenvalues for the two-level system[§]

$$\lambda_{\pm} = r\cos(\theta) \pm \sqrt{k^2 - r^2\sin^2(\theta)}, \tag{3.1.2}$$

where $\pm$ represents the two-levels of energy. From the eigenvalues equation we observe that when $r^2\sin^2(\theta) < k^2$ the energy eigenvalues are real and the symmetry is unbroken. On the other case, when $r^2\sin^2(\theta) > k^2$ the energy eigenvalues are complex and the symmetry is broken. Also, equation (3.1.2) shows the same eigenvalues as equation (2.4.4) therefore, the matrix H_b is similar to matrix H_a. In order to define the $\mathcal{PT}$ inner product we need to find the eigenstates of the system. To find the eigenstates, we replace the

[§]See Appendix B for exact calculations.

eigenvalues in the determinant matrix as follows

$$\begin{pmatrix} re^{+(i\theta)} - \lambda_{(+)} & k \\ k & re^{-(i\theta)} - \lambda_{(+)} \end{pmatrix} = 0,$$

$$\begin{pmatrix} re^{+(i\theta)} - (r\cos(\theta) + \sqrt{k^2 - r^2\sin^2(\theta)}) & k \\ k & re^{-(i\theta)} - (r\cos(\theta) + \sqrt{k^2 - r^2\sin^2(\theta)}) \end{pmatrix} = 0,$$

where the first position on the diagonal is obtained by

$r(\cos(\theta) + i\sin(\theta)) - (r\cos(\theta) + \sqrt{k^2 - r^2\sin^2(\theta)})$

$\Rightarrow r\cos(\theta) + ir\sin(\theta) - r\cos(\theta) - \sqrt{k^2 - r^2\sin^2(\theta)}$

$\Rightarrow ir\sin(\theta) - \sqrt{k^2 - r^2\sin^2(\theta)}$

and the second position on the diagonal is obtained by

$r(\cos(\theta) - i\sin(\theta)) - (r\cos(\theta) + \sqrt{k^2 - r^2\sin^2(\theta)})$

$\Rightarrow r\cos(\theta) - ir\sin(\theta) - r\cos(\theta) - \sqrt{k^2 - r^2\sin^2(\theta)}$

$\Rightarrow -ir\sin(\theta) - \sqrt{k^2 - r^2\sin^2(\theta)},$

then we have

$$\begin{pmatrix} ir\sin(\theta) - \sqrt{k^2 - r^2\sin^2(\theta)} & k \\ k & -ir\sin(\theta) - \sqrt{k^2 - r^2\sin^2(\theta)}) \end{pmatrix} = 0$$

$$\Rightarrow \begin{pmatrix} \frac{1}{k}(ir\sin(\theta) - \sqrt{k^2 - r^2\sin^2(\theta)}) & 1 \\ 1 & \frac{1}{k}(-ir\sin(\theta) - \sqrt{k^2 - r^2\sin^2(\theta)}) \end{pmatrix} = 0$$

$$\Rightarrow \begin{pmatrix} \frac{1}{k}(ir\sin(\theta)) - \sqrt{1-\frac{r^2}{k^2}\sin^2(\theta)} & 1 \\ 1 & \frac{1}{k}(-ir\sin(\theta)) - \sqrt{1-\frac{r^2}{k^2}\sin^2(\theta)} \end{pmatrix} = 0$$

$$\Rightarrow \begin{pmatrix} 1 & \frac{1}{k}(-ir\sin(\theta)) - \sqrt{1-\frac{r^2}{k^2}\sin^2(\theta)} \\ \frac{1}{k}(ir\sin(\theta)) - \sqrt{1-\frac{r^2}{k^2}\sin^2(\theta)} & 1 \end{pmatrix} = 0$$

$$\Rightarrow \begin{pmatrix} 1 & \frac{1}{k}(-ir\sin(\theta)) - \sqrt{1-\frac{r^2}{k^2}\sin^2(\theta)} \\ 0 & 0 \end{pmatrix} = 0$$

$$\Rightarrow \begin{pmatrix} 1 & -e^{(i\alpha)} \\ 0 & 0 \end{pmatrix} = 0.$$

We used the Euler formula (3.0.1) and the trigonometric equation $\cos^2(\theta) + \sin^2\theta = 1$, in order to define $\cos(\alpha) = \frac{r}{k}\cos(\theta) = \sqrt{1-\frac{r^2}{k^2}\sin^2(\theta)}$ and $i\sin(\alpha) = \frac{r}{k}i\sin(\theta)$. Then, $e^{(i\alpha)} = \cos(\alpha) + i\sin(\alpha)$.

If $x_2 = e^{-(i\alpha)}$, then the eigenstate is given by

$$|+\rangle = \begin{pmatrix} 1 \\ +e^{-(i\alpha)} \end{pmatrix}.$$

Using the second eigenvalue we arrive at the following determinant matrix

$$\begin{pmatrix} \frac{1}{k}(ir\sin(\theta)) + \sqrt{1-\frac{r^2}{k^2}\sin^2(\theta)} & 1 \\ 1 & \frac{1}{k}(-ir\sin(\theta)) + \sqrt{1-\frac{r^2}{k^2}\sin^2(\theta)} \end{pmatrix} = 0$$

$$\Rightarrow \begin{pmatrix} 1 & \frac{1}{k}(-ir\sin(\theta)) + \sqrt{1 - \frac{r^2}{k^2}\sin^2(\theta)} \\ \frac{1}{k}(ir\sin(\theta)) + \sqrt{1 - \frac{r^2}{k^2}\sin^2(\theta)} & 1 \end{pmatrix} = 0$$

$$\Rightarrow \begin{pmatrix} 1 & \frac{1}{k}(-ir\sin(\theta)) + \sqrt{1 - \frac{r^2}{k^2}\sin^2(\theta)} \\ 0 & 0 \end{pmatrix} = 0$$

$$\Rightarrow \begin{pmatrix} 1 & e^{-(i\alpha)} \\ 0 & 0 \end{pmatrix} = 0.$$

If $x_2 = -e^{(i\alpha)}$, then the eigenstate is given by

$$|-\rangle = \begin{pmatrix} 1 \\ -e^{+(i\alpha)} \end{pmatrix}.$$

We know that the eigenstates of the system denoted as $|\pm\rangle$ are as follows

$$|\pm\rangle = \begin{pmatrix} 1 \\ \pm e^{\mp(i\alpha)} \end{pmatrix}.$$

We normalize the eigenstates up to a phase using the following relation

$$\phi_n(x) = e^{\pm i(\frac{\alpha}{2})}\psi_n(x), \tag{3.1.3}$$

where $\psi_n(x)$ are the eigenstates of the system, then the normalized eigenstates are as follows

$$|\epsilon_+\rangle = e^{i(\frac{\alpha}{2})} \begin{pmatrix} 1 \\ e^{-i(\alpha)} \end{pmatrix},$$

$$|\epsilon_+\rangle = \frac{1}{\sqrt{2\cos(\alpha)}} \begin{pmatrix} e^{i(\frac{\alpha}{2})} \\ e^{-i(\frac{\alpha}{2})} \end{pmatrix},$$

$$|\epsilon_-\rangle = e^{-i(\frac{\alpha}{2})} \begin{pmatrix} 1 \\ -e^{i(\alpha)} \end{pmatrix},$$

$$|\epsilon_-\rangle = \frac{i}{\sqrt{2\cos(\alpha)}} \begin{pmatrix} e^{-i(\frac{\alpha}{2})} \\ -e^{i(\frac{\alpha}{2})} \end{pmatrix}.$$

The normalization constant is obtained using the following relation

$$\langle L_n | R_m \rangle = \delta_{nm}, \tag{3.1.4}$$

where L_n are the left eigenvectors,[‡] R_m are the right eigenvectors and δ_{nm} is the Dirac delta function. Then,

$$A^2 \begin{pmatrix} e^{+(i\alpha)} & 1 \end{pmatrix} * \begin{pmatrix} 1 \\ e^{-(i\alpha)} \end{pmatrix} = 1$$

$$\Rightarrow A^2(e^{-(i\alpha)} + e^{(i\alpha)}) = 1$$

$$\Rightarrow A^2 2\cos(\alpha) = 1$$

$$\Rightarrow A = \frac{1}{\sqrt{2\cos(\alpha)}},$$

where the left eigenvectors are given by

$$|L_+\rangle = \begin{pmatrix} e^{-(i\alpha)} \\ 1 \end{pmatrix}$$

and

[‡]See Appendix A.

$$|L_-\rangle = \begin{pmatrix} -e^{(i\alpha)} \\ 1 \end{pmatrix}.$$

The $\mathcal{PT}$ inner product is defined as

$$(u, v) = (\mathcal{PT}u) \cdot v, \tag{3.1.5}$$

where u and v are the normalized eigenstates. Notice that the last definition follows from equation (2.5.12). We observe that the inner product is not positive definite as shown below. We show that the $\mathcal{PT}$ inner product can be positive, negative or zero.

$$(\epsilon_\pm|\epsilon_\pm) = \pm 1, \quad and \quad (\epsilon_\pm|\epsilon_\mp) = 0. \tag{3.1.6}$$

(I) Positive inner product is given by $(\epsilon_+|\epsilon_+) = (\mathcal{PT}\epsilon_+|\epsilon_+) = +1$,

where

$$(\mathcal{PT}\epsilon_+) = \frac{1}{\sqrt{2\cos(\alpha)}} \begin{pmatrix} e^{i(\frac{\alpha}{2})} \\ e^{-i(\frac{\alpha}{2})} \end{pmatrix}.$$

Then,

$$(\epsilon_+|\epsilon_+) = \left(\frac{1}{\sqrt{2\cos(\alpha)}}\right)^2 \begin{pmatrix} e^{i(\frac{\alpha}{2})} & e^{-i(\frac{\alpha}{2})} \end{pmatrix} * \begin{pmatrix} e^{i(\frac{\alpha}{2})} \\ e^{-i(\frac{\alpha}{2})} \end{pmatrix},$$

$$(\epsilon_+|\epsilon_+) = \frac{1}{2\cos(\alpha)} * (e^{(i\alpha)} + e^{-(i\alpha)}) = \frac{2\cos(\alpha)}{2\cos(\alpha)} = 1.$$

(II) Negative inner product is given by $(\epsilon_-|\epsilon_-) = (\mathcal{PT}\epsilon_-|\epsilon_-) = -1$,

where

$$(\mathcal{PT}\epsilon_-) = \frac{i}{\sqrt{2\cos(\alpha)}} \begin{pmatrix} -e^{-i(\frac{\alpha}{2})} \\ e^{i(\frac{\alpha}{2})} \end{pmatrix}.$$

Then,

$$(\epsilon_-|\epsilon_-) = \left(\frac{1}{\sqrt{2\cos(\alpha)}}\right)^2 - i * i \begin{pmatrix} -e^{-i(\frac{\alpha}{2})} & e^{i(\frac{\alpha}{2})} \end{pmatrix} * \begin{pmatrix} e^{-i(\frac{\alpha}{2})} \\ -e^{i(\frac{\alpha}{2})} \end{pmatrix},$$

$$(\epsilon_-|\epsilon_-) = \frac{1}{2\cos(\alpha)}(-e^{-(i\alpha)} + -e^{(i\alpha)}) = \frac{1 * -2\cos(\alpha)}{2\cos(\alpha)} = -1.$$

(III) If the inner product is zero, then $(\epsilon_+|\epsilon_-) = (\mathcal{PT}\epsilon_+|\epsilon_-) = 0$,

where

$$(\mathcal{PT}\epsilon_+) = \frac{1}{2\cos(\alpha)} \begin{pmatrix} e^{i(\frac{\alpha}{2})} \\ e^{-i(\frac{\alpha}{2})} \end{pmatrix}.$$

Then,

$$(\epsilon_+|\epsilon_-) = \frac{i}{2\cos(\alpha)} \begin{pmatrix} e^{i(\frac{\alpha}{2})} & e^{-i(\frac{\alpha}{2})} \end{pmatrix} * \begin{pmatrix} e^{-i(\frac{\alpha}{2})} \\ -e^{i(\frac{\alpha}{2})} \end{pmatrix},$$

$$(\epsilon_+|\epsilon_-) = \frac{i}{2\cos(\alpha)} * (1 - 1) = 0.$$

As well as $(\epsilon_-|\epsilon_+) = (\mathcal{PT}\epsilon_-|\epsilon_+) = 0$,

where

$$(\mathcal{PT}\epsilon_-) = \frac{-i}{2\cos(\alpha)} \begin{pmatrix} -e^{-i(\frac{\alpha}{2})} \\ e^{i(\frac{\alpha}{2})} \end{pmatrix}.$$

Then,

$$(\epsilon_-|\epsilon_+) = \frac{-i}{2\cos(\alpha)} \begin{pmatrix} -e^{-i(\frac{\alpha}{2})} & e^{i(\frac{\alpha}{2})} \end{pmatrix} * \begin{pmatrix} e^{i(\frac{\alpha}{2})} \\ e^{-i(\frac{\alpha}{2})} \end{pmatrix},$$

$$(\epsilon_-|\epsilon_+) = \frac{-i}{2\cos(\alpha)} * (-1+1) = 0.$$

3.2 The $\mathcal{CPT}$ Inner Product

As predicted for the theory the $\mathcal{PT}$ inner product is not positive definite, we need to construct the $\mathcal{C}$ operator in order to define a positive definite inner product [8]. The $\mathcal{C}$ operator is defined by the following equation

$$\mathcal{C}(x,y) = \sum_{n=0}^{\infty} \phi_n(x)\phi_n(y). \tag{3.2.1}$$

In the specific case of the two-level system Hamiltonian the $\mathcal{C}$ operator is constructed as follows

$$\mathcal{C} = \frac{1}{2\cos(\alpha)} \begin{pmatrix} e^{i(\frac{\alpha}{2})} \\ e^{-i(\frac{\alpha}{2})} \end{pmatrix} * \begin{pmatrix} e^{i(\frac{\alpha}{2})} & e^{-i(\frac{\alpha}{2})} \end{pmatrix} + \frac{i^2}{2\cos(\alpha)} \begin{pmatrix} e^{-i(\frac{\alpha}{2})} \\ -e^{i(\frac{\alpha}{2})} \end{pmatrix} * \begin{pmatrix} e^{-i(\frac{\alpha}{2})} & -e^{i(\frac{\alpha}{2})} \end{pmatrix}$$

$$\Rightarrow \mathcal{C} = \frac{1}{2\cos(\alpha)} \begin{pmatrix} e^{(i\alpha)} & 1 \\ 1 & e^{-(i\alpha)} \end{pmatrix} + \frac{-1}{2\cos(\alpha)} \begin{pmatrix} e^{-(i\alpha)} & -1 \\ -1 & e^{+(i\alpha)} \end{pmatrix}$$

$$\Rightarrow \mathcal{C} = \frac{1}{2\cos(\alpha)} \begin{pmatrix} e^{(i\alpha)} & 1 \\ 1 & e^{-(i\alpha)} \end{pmatrix} + \frac{1}{2\cos(\alpha)} \begin{pmatrix} -e^{-(i\alpha)} & 1 \\ 1 & -e^{+(i\alpha)} \end{pmatrix}$$

$$\Rightarrow \mathcal{C} = \frac{1}{2\cos(\alpha)} \begin{pmatrix} e^{(i\alpha)} - e^{-(i\alpha)} & 2 \\ 2 & e^{-(i\alpha)} - e^{(i\alpha)} \end{pmatrix}$$

$$\Rightarrow \mathcal{C} = \frac{1}{2\cos(\alpha)} \begin{pmatrix} 2i\sin(\alpha) & 2 \\ 2 & -2i\sin(\alpha) \end{pmatrix}$$

$$\Rightarrow \mathcal{C} = \frac{1}{\cos(\alpha)} \begin{pmatrix} i\sin(\alpha) & 1 \\ 1 & -i\sin(\alpha) \end{pmatrix}.$$

Now that we had constructed the $\mathcal{C}$ operator of a two-level system Hamiltonian we show that $\mathcal{C}^2 = I$ as stated in equation (2.5.16).

$$\mathcal{C}^2 = \frac{1}{\cos^2(\alpha)} \begin{pmatrix} i\sin(\alpha) & 1 \\ 1 & -i\sin(\alpha) \end{pmatrix} * \begin{pmatrix} i\sin(\alpha) & 1 \\ 1 & -i\sin(\alpha) \end{pmatrix}$$

$$\Rightarrow \mathcal{C}^2 = \frac{1}{\cos^2(\alpha)} \begin{pmatrix} i^2\sin^2(\alpha) + 1 & i\sin(\alpha) - i\sin(\alpha) \\ i\sin(\alpha) - i\sin(\alpha) & 1 + i^2\sin^2(\alpha) \end{pmatrix}$$

$$\Rightarrow \mathcal{C}^2 = \frac{1}{\cos^2(\alpha)} \begin{pmatrix} (-1)\sin^2(\alpha) + 1 & 0 \\ 0 & 1 + (-1)\sin^2(\alpha) \end{pmatrix}$$

$$\Rightarrow \mathcal{C}^2 = \frac{1}{\cos^2(\alpha)} \begin{pmatrix} \cos^2(\alpha) & 0 \\ 0 & \cos^2(\alpha) \end{pmatrix}$$

$$\Rightarrow \mathcal{C}^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Using the $\mathcal{C}$ operator we define the new inner product as follows

$$\langle u|v\rangle = (\mathcal{CPT}u) \cdot v, \tag{3.2.2}$$

where u and v are the normalized eigenstates. With this definition the inner product is positive definitive since $\langle \epsilon_\pm | \epsilon_\pm \rangle = 1$. We will show this result explicitly since the inner

product constructed with the $\mathcal{C}$ operator is specific to the non-Hermitian $\mathcal{PT}$ symmetry theory.

(I) We will show that the inner product of the ϵ_+ eigenvector with itself is positive. Then, $\langle\epsilon_+|\epsilon_+\rangle = (\mathcal{CPT}\epsilon_+)\cdot\epsilon_+ = 1$,

$$\langle\epsilon_+|\epsilon_+\rangle = \frac{1}{\cos(\alpha)}\frac{1}{\sqrt{2\cos(\alpha)}}\begin{pmatrix} i\sin(\alpha) & 1 \\ 1 & -i\sin(\alpha)\end{pmatrix} * \begin{pmatrix} e^{i(\frac{\alpha}{2})} \\ e^{-i(\frac{\alpha}{2})}\end{pmatrix}$$

$$= \frac{1}{\cos(\alpha)}\frac{1}{\sqrt{2\cos(\alpha)}}\begin{pmatrix} i\sin(\alpha)e^{i(\frac{\alpha}{2})} + e^{-i(\frac{\alpha}{2})} \\ e^{i(\frac{\alpha}{2})} - i\sin(\alpha)e^{-i(\frac{\alpha}{2})}\end{pmatrix}$$

$$= \frac{\sec^2(\alpha)}{2}\begin{pmatrix} i\sin(\alpha)e^{i(\frac{\alpha}{2})} + e^{-i(\frac{\alpha}{2})}, & e^{i(\frac{\alpha}{2})} - i\sin(\alpha)e^{-i(\frac{\alpha}{2})}\end{pmatrix} * \begin{pmatrix} e^{i(\frac{\alpha}{2})} \\ e^{-i(\frac{\alpha}{2})}\end{pmatrix}$$

$$= \frac{\sec^2(\alpha)}{2}\begin{pmatrix} i\sin(\alpha)e^{i(\frac{\alpha}{2})}e^{i(\frac{\alpha}{2})} + e^{-i(\frac{\alpha}{2})}e^{i(\frac{\alpha}{2})} + e^{i(\frac{\alpha}{2})}e^{-i(\frac{\alpha}{2})} - i\sin(\alpha)e^{-i(\frac{\alpha}{2})}e^{-i(\frac{\alpha}{2})}\end{pmatrix}$$

$$= \frac{\sec^2(\alpha)}{2}\begin{pmatrix} i\sin(\alpha)e^{i(\alpha)} + 1 + 1 - i\sin(\alpha)e^{-i(\alpha)}\end{pmatrix}$$

$$= \frac{\sec^2(\alpha)}{2}\begin{pmatrix} 2 + i\sin(\alpha)(e^{i(\alpha)} - e^{-i(\alpha)})\end{pmatrix}$$

$$= \frac{\sec^2(\alpha)}{2}\begin{pmatrix} 2 - 2\sin^2(\alpha)\end{pmatrix}$$

$$= \frac{\sec^2(\alpha)}{2}\begin{pmatrix} 2\cos^2(\alpha)\end{pmatrix}$$

$$= \sec^2(\alpha)\ \cos^2(\alpha) = 1.$$

Therefore, $(\mathcal{CPT}\epsilon_+)\cdot\epsilon_+ = 1$.

(II) We will show that the inner product of the ϵ_- eigenvector with itself is positive. Then,

$\langle\epsilon_-|\epsilon_-\rangle = (\mathcal{CPT}\epsilon_-)\cdot\epsilon_- = 1,$

$$\langle\epsilon_-|\epsilon_-\rangle = \frac{1}{\cos(\alpha)}\frac{1}{\sqrt{2\cos(\alpha)}}\begin{pmatrix} i\sin(\alpha) & 1 \\ 1 & -i\sin(\alpha)\end{pmatrix} * \begin{pmatrix} -e^{-i(\frac{\alpha}{2})} \\ e^{i(\frac{\alpha}{2})}\end{pmatrix}$$

$$= \frac{1}{\cos(\alpha)}\frac{1}{\sqrt{2\cos(\alpha)}}\begin{pmatrix} -i\sin(\alpha)e^{-i(\frac{\alpha}{2})} + e^{i(\frac{\alpha}{2})} \\ -e^{-i(\frac{\alpha}{2})} - i\sin(\alpha)e^{i(\frac{\alpha}{2})}\end{pmatrix}$$

$$= \frac{\sec^2(\alpha)}{2}\begin{pmatrix} -i\sin(\alpha)e^{-i(\frac{\alpha}{2})} + e^{i(\frac{\alpha}{2})}, & -e^{-i(\frac{\alpha}{2})} - i\sin(\alpha)e^{i(\frac{\alpha}{2})}\end{pmatrix} * \begin{pmatrix} e^{-i(\frac{\alpha}{2})} \\ -e^{i(\frac{\alpha}{2})}\end{pmatrix}$$

$$= \frac{\sec^2(\alpha)}{2}\begin{pmatrix} -i\sin(\alpha)e^{-i(\alpha)} + 1 + 1 + i\sin(\alpha)e^{i(\alpha)}\end{pmatrix}$$

$$= \frac{\sec^2(\alpha)}{2}\begin{pmatrix} 2 + i\sin(\alpha)(e^{i(\alpha)} - e^{-i(\alpha)})\end{pmatrix}$$

$$= \frac{\sec^2(\alpha)}{2}\begin{pmatrix} 2 - 2\sin^2(\alpha)\end{pmatrix}$$

$$= \frac{\sec^2(\alpha)}{2}\ 2\cos^2(\alpha) = 1.$$

Therefore, $(\mathcal{CPT}\epsilon_-)\cdot\epsilon_- = 1$.

4 Solution to Non-Hermitian Hamiltonians

4.1 Eigenvalues of H Using WKB and Semi-Classical Approximation

In order to find the eigenvalues of $\mathcal{H} = p^2 + x^2(ix)^\varepsilon$, we need to solve the equation

$$\hat{\mathcal{H}}\psi = E\psi. \tag{4.1.1}$$

It is necessary to rewrite $\mathcal{H}$ as a differential equation in a coordinate space, then

$$\hat{x} \to x, \qquad \hat{p} = -i\hbar\frac{\partial}{\partial x}, \tag{4.1.2}$$

treating the variable x as a complex variable and assuming $\hbar = 1$ then, the Schrödinger eigenvalue problem is as follows

$$\left[\left(-i\hbar\frac{\partial}{\partial x}\right)^2 + x^2(ix)^\varepsilon\right]\psi(x) = E\psi(x), \tag{4.1.3}$$

$$-\psi''(x) + x^2(ix)^\varepsilon\psi(x) = E\psi(x). \tag{4.1.4}$$

Since the last equation does not have an exact solution for arbitrary ε it is necessary to use the WKB (Wentzel Kramers Brillouin) method to find out the possible asymptotic behaviors of its solutions [1].

The WKB method is use for approximating the solution of a differential equation. In order to do so the highest derivative in the equation is multiplied by a small parameter ς. The parameter sigma belongs to the real numbers [13]. Then, consider the following differential equation

$$\varsigma^2 y'' = Q(x)y, \quad Q(x) \neq 0. \tag{4.1.5}$$

In order to solve equation (4.1.5) we use an ansatz solution of the form

$$y(x) \sim \exp\left[\frac{1}{\delta}\sum_{n=0}^{\infty}\delta^n S_n(x)\right], \quad \delta \to 0, \tag{4.1.6}$$

where $S_n(x)$ is a series in power of δ and $\frac{1}{\delta}$ is an asymptotic scaling. If we take the first and second derivatives of $y(x)$ we have

$$y'(x) \sim \left(\frac{1}{\delta}\sum_{n=0}^{\infty}\delta^n S_n'(x)\right)\exp\left(\frac{1}{\delta}\sum_{n=0}^{\infty}\delta^n S_n(x)\right), \quad \delta \to 0, \tag{4.1.7}$$

$$y''(x) \sim \left[\frac{1}{\delta^2}\left(\sum_{n=0}^{\infty}\delta^n S_n'(x)\right)^2 + \frac{1}{\delta}\sum_{n=0}^{\infty}\delta^n S_n''(x)\right]\exp\left(\frac{1}{\delta}\sum_{n=0}^{\infty}\delta^n S_n(x)\right), \quad \delta \to 0. \tag{4.1.8}$$

Next, we substitute equation (4.1.8) and (4.1.6) into equation (4.1.5) and cancel the exponential factor as follows

$$\frac{\varsigma^2}{\delta^2}S_0'^2(x) + \frac{2\varsigma^2}{\delta}S_0'(x)S_1'(x) + \frac{\varsigma^2}{\delta}S_0''(x) + \ldots = Q(x). \tag{4.1.9}$$

By dominant balance the first term of equation (4.1.9) must be equal to $Q(x)$; therefore, δ is proportional to ς choosing $\varsigma = \delta$ and comparing power of ς we have

$$S_0'^2(x) = Q(x), \tag{4.1.10}$$

$$2S_0'(x)S_1'(x) + S_0''(x) = 0, \tag{4.1.11}$$

$$2S_0'(x)S_n'(x) + S_{n-1}''(x) + \sum_{j=1}^{n-1}S_j'(x)S_{n-j}'(x) = 0 \quad n \geq 2. \tag{4.1.12}$$

The solution of equation (4.1.10) is as follows

$$S_0'^2(x) = Q(x)$$

$$\Rightarrow S_0'(x) = \sqrt{Q(x)}$$

$$\Rightarrow S_0(x) = \pm \int^x \sqrt{Q(t)}dt. \tag{4.1.13}$$

The solution of equation (4.1.11) is as follows

$$2S_0'(x)S_1'(x) + S_0''(x) = 0$$

$$\Rightarrow S_1'(x) = -\frac{S_0''(x)}{2S_0'(x)},$$

where $S_0'(x) = \sqrt{Q(x)}$ and $S_0''(x) = \frac{1}{2}Q(x)^{-\frac{1}{2}}$

$$\Rightarrow S_1'(x) = -\frac{1}{4}\frac{1}{Q(x)}$$

and

$$S_1(x) = -\frac{1}{4}\ln Q(x). \tag{4.1.14}$$

Then, the general solution of equation (4.1.5) is a combination of the two solutions

$$y(x) \sim c_1 Q^{-\frac{1}{4}}(x) \exp\left[\frac{1}{\varsigma}\int_a^x dt\sqrt{Q(t)}\right] + c_2 Q^{-\frac{1}{4}}(x) \exp\left[-\frac{1}{\varsigma}\int_a^x dt\sqrt{Q(t)}\right], \varsigma \to 0. \tag{4.1.15}$$

The last equation is the general solution of the Schrödinger equation obtained by the WKB approximation.

Now that we solved the Schrödinger equation using WKB, we need to apply semi-classical techniques to find the spectrum of equation (1.0.7). In order to do so we use classical theory of turning points and we apply WKB.

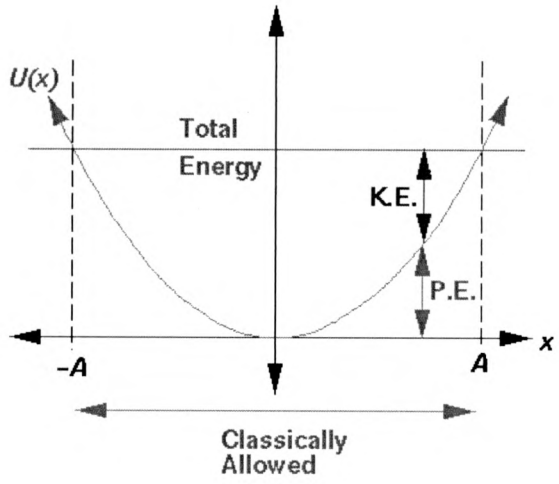

Figure 3: The graph shows the classically allowed region defined between turning points $-A$ and A. We observe the potential $U(x)$ vs. x.

We define the classical turning point as the point at which the potential energy V is equal to the total energy E, as seen on Figure 3. If $E > V$ then a classical particle has a non-zero kinetic energy and is allowed to move freely, if $E < V$ then the classical particle is not allowed in the region after V but a quantum particle can tunnel to this region. The WKB method implements this point of view and matches the wave function in the different regions defined by the turning points.

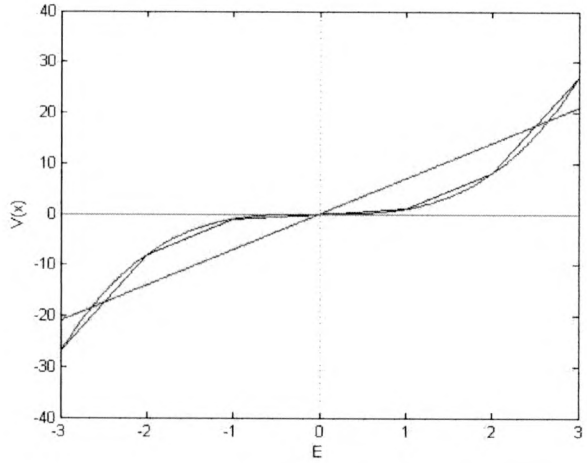

Figure 4: One turning point approximation. The graph is centered at the point (0,0) where the total energy is equal to the potential. Notice this is described by point A in Figure 3.

First, we analyze the solution of WKB on one turning point as seen on Figure 4. Suppose

that we center the turning point at $(0,0)$ then the potential V has three regions well defined: region I when $x > 0$, region II where x is near to 0 and region III where $x < 0$. To find the wave function of each region we use WKB to solve the following equation

$$\varsigma'' y''(x) = Q(x)y. \tag{4.1.16}$$

where $Q(x) = V(x) - E$, without loss of generality we present the solution on the three regions.

Region I

$$y(x) \sim C\frac{1}{(Q(x))^{\frac{1}{4}}} \exp\left[-\frac{1}{\varsigma}\int_0^x dt\sqrt{Q(t)}\right] \quad x > 0 \quad as \quad \varsigma \to 0. \tag{4.1.17}$$

Region II

$$y(x) \sim C\frac{2\sqrt{\pi}}{(a\varsigma)^{\frac{1}{6}}} Ai\left(\frac{xa^{\frac{1}{3}}}{\varsigma^{\frac{2}{3}}}\right) \quad << 1 \quad as \quad \varsigma \to 0. \tag{4.1.18}$$

Region III

$$y(x) \sim 2C\frac{1}{(-Q(x))^{\frac{1}{4}}} \sin\left[\frac{1}{\varsigma}\int_x^0 dt\sqrt{-Q(t)} + \frac{\pi}{4}\right] \quad x < 0 \quad \varsigma \to 0. \tag{4.1.19}$$

Notice that in order for the results to be true where region I overlaps region II, the two solutions have to be equal. The same equality condition applies to regions II and III.

Now that we know the solution to one turning point problem we extend the answer to a two turning point problem. Then, we define three new regions for the second turning point such as region I-B where $x > 0$, region II-B where x is near to 0 and region III-B where $x < 0$. This turning point is located at $x = -A = \alpha$ which is the one to the left side of Figure 3 and the other one is located at $x = A = \beta$ which is the one to the right

side of Figure 3. Therefore, the turning point at A defines region I, II and III with the corresponding wave function. The turning point at $x = -A$ defines regions I-B, II-B and III-B with the corresponding wave function. Notice that all the limits of integration run to the positive values of x.

Region I

$$y(x) \sim C\frac{1}{(Q(x))^{\frac{1}{4}}}\exp\left[-\frac{1}{\varsigma}\int_{\beta}^{x} dt\sqrt{Q(t)}\right] \quad x > 0 \quad as \quad \varsigma \to 0. \tag{4.1.20}$$

Region II

$$y(x) \sim C\frac{2\sqrt{\pi}}{(a\varsigma)^{\frac{1}{6}}}Ai\left(\frac{xa^{\frac{1}{3}}}{\varsigma^{\frac{2}{3}}}\right) \quad << 1 \quad as \quad \varsigma \to 0. \tag{4.1.21}$$

Region III

$$y(x) \sim 2C\frac{1}{(-Q(x))^{\frac{1}{4}}}\sin\left[\frac{1}{\varsigma}\int_{x}^{\beta} dt\sqrt{-Q(t)} + \frac{\pi}{4}\right] \quad x < 0 \quad \varsigma \to 0. \tag{4.1.22}$$

Region I-B

$$y(x) \sim D\frac{1}{(Q(x))^{\frac{1}{4}}}\exp\left[-\frac{1}{\varsigma}\int_{x}^{\alpha} dt\sqrt{Q(t)}\right] \quad \varsigma \to 0 \quad as \quad x \to -\infty. \tag{4.1.23}$$

Region II-B

$$y(x) \sim D\frac{2\sqrt{\pi}}{(a\varsigma)^{\frac{1}{6}}}Ai\left(\frac{xa^{\frac{1}{3}}}{\varsigma^{\frac{2}{3}}}\right) \quad << 1 \quad as \quad \varsigma \to 0. \tag{4.1.24}$$

Region III-B

$$y(x) \sim 2D\frac{1}{(-Q(x))^{\frac{1}{4}}}\sin\left[\frac{1}{\varsigma}\int_{\alpha}^{x} dt\sqrt{-Q(t)} + \frac{\pi}{4}\right] \quad as \quad \varsigma \to 0. \tag{4.1.25}$$

Now that we have the solution to the two turning points, we need the solution to be valid in the classical region as defined by regions III and III-B. We need to match them to find a solution to the problem. Therefore,

$$2D\frac{1}{(-Q(x))^{\frac{1}{4}}}\sin\left[\frac{1}{\varsigma}\int_{\alpha}^{x} dt\sqrt{-Q(t)} + \frac{\pi}{4}\right] \sim 2C\frac{1}{(-Q(x))^{\frac{1}{4}}}\sin\left[\frac{1}{\varsigma}\int_{x}^{\beta} dt\sqrt{-Q(t)} + \frac{\pi}{4}\right], \tag{4.1.26}$$

then we work on the left side of equation (4.1.26) in order to make it look like the right side of equation. Therefore, we add an integral from α to β and we subtract the integral from x to β. Then, we multiply it by -1 since sine is an odd function, we add $\frac{\pi}{4}$ to the integral from x to β and subtract the same amount, then

$$y(x) \sim 2D\frac{1}{(-Q(x))^{\frac{1}{4}}}\sin\left[\frac{1}{\varsigma}\int_{\alpha}^{\beta} dt\sqrt{-Q(t)} - \frac{1}{\varsigma}\int_{x}^{\beta} dt\sqrt{-Q(t)} + \frac{\pi}{4}\right]$$

$$\Rightarrow y(x) \sim -\left[2D\frac{1}{(-Q(x))^{\frac{1}{4}}}\sin\left[\frac{1}{\varsigma}\int_{\alpha}^{\beta} dt\sqrt{-Q(t)} - \frac{1}{\varsigma}\int_{x}^{\beta} dt\sqrt{-Q(t)} + \frac{\pi}{4}\right]\right]$$

$$\Rightarrow y(x) \sim -2D\frac{1}{(-Q(x))^{\frac{1}{4}}}\sin\left[-\frac{1}{\varsigma}\int_{\alpha}^{\beta} dt\sqrt{-Q(t)} + \frac{1}{\varsigma}\int_{x}^{\beta} dt\sqrt{-Q(t)} - \frac{\pi}{4}\right]$$

$$\Rightarrow y(x) \sim -2D\frac{1}{(-Q(x))^{\frac{1}{4}}}\sin\left[-\frac{1}{\varsigma}\int_{\alpha}^{\beta} dt\sqrt{-Q(t)} + \frac{1}{\varsigma}\int_{x}^{\beta} dt\sqrt{-Q(t)} + \frac{\pi}{4} - \frac{\pi}{4} - \frac{\pi}{4}\right]$$

$$\Rightarrow y(x) \sim -2D\frac{1}{(-Q(x))^{\frac{1}{4}}}\sin\left[-\frac{1}{\varsigma}\int_{\alpha}^{\beta} dt\sqrt{-Q(t)}+\frac{1}{\varsigma}\int_{x}^{\beta} dt\sqrt{-Q(t)}+\frac{\pi}{4}-\frac{\pi}{2}\right]$$

$$\Rightarrow y(x) \sim -2D\frac{1}{(-Q(x))^{\frac{1}{4}}}\sin\left[\underbrace{-\frac{1}{\varsigma}\int_{\alpha}^{\beta} dt\sqrt{-Q(t)}-\frac{\pi}{2}}_{\kappa}+\frac{1}{\varsigma}\int_{x}^{\beta} dt\sqrt{-Q(t)}+\frac{\pi}{4}\right].$$

Therefore, equations (4.1.22) and (4.1.25) are equal if the constants are equal and if the constraint κ is equal to 0, then

$$\sin\left(-\frac{1}{\varsigma}\int_{\alpha}^{\beta} dt\sqrt{-Q(t)}-\frac{\pi}{2}\right)=0$$

$$\Rightarrow (-1)\sin\left(-\frac{1}{\varsigma}\int_{\alpha}^{\beta} dt\sqrt{-Q(t)}-\frac{\pi}{2}\right)=0$$

$$\Rightarrow +\frac{1}{\varsigma}\int_{\alpha}^{\beta} dt\sqrt{-Q(t)}+\frac{\pi}{2}=n\pi \quad n=1,2,3,...$$

$$\Rightarrow \frac{1}{\varsigma}\int_{\alpha}^{\beta} dt\sqrt{-Q(t)}=\left(n-\frac{1}{2}\right)\pi \quad n=1,2,3,...$$

Then, shift n by 1 and we have the following constraint where the solution of the two turning points is valid.

$$\boxed{\frac{1}{\varsigma}\int_{\alpha}^{\beta} dt\sqrt{-Q(t)}=\left(n+\frac{1}{2}\right)\pi, \quad n=0,1,2,3,..., \quad \varsigma\to 0.} \tag{4.1.27}$$

Notice the last solution is known as the Bohr-Sommerfeld quantization rule [4]. Using this constraint means that the constants are equal if $C=(-1)^n D$.

4.2 Wedges

To solve equations (1.0.6) and (1.0.7) we use the result of the WKB approximation, then, we have the solutions of the form

$$y(x) \sim exp \pm \left[\int^{x} ds \sqrt{V(s)} \right], \tag{4.2.1}$$

where $V(s)$ is a function of x. With the following boundary condition imposed on the equations $\psi(x) \to 0$ as $|x| \to \infty$. If $\varepsilon = 0$ in equation (1.0.7) we have the harmonic oscillator and the asymptotic behavior of the solutions as follows

$$y(x) \sim exp \pm \left[\frac{1}{2} x^2 \right]. \tag{4.2.2}$$

We keep the solution with the negative sign because the eigenfunction has to be square integrable. The solutions (4.2.2) are Gaussian like for large $|x|$ then, if equation (4.2.2) vanishes exponentially for large $|x|$ in the real axis, they must also vanish in the complex plane, forming two wedges at an angle of $\frac{\pi}{2}$. These two wedges are called Stokes wedges, as seen in Figure 5 and the solution of Hamiltonian $\mathcal{H}$ is valid inside these wedges [9, 11].

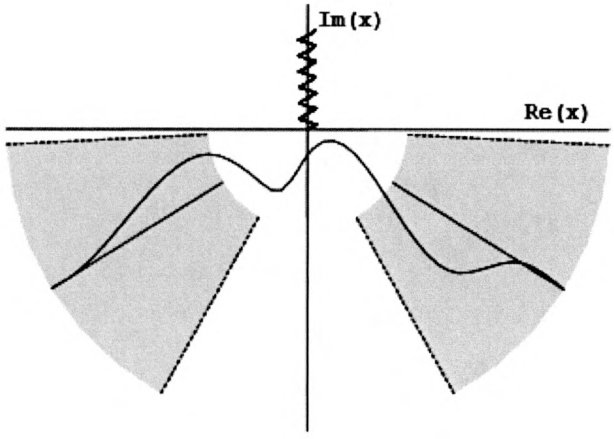

Figure 5: Stokes wedges in the complex x plane containing the contour on which the eigenvalue problem for the differential equation (4.1.3) has a solution, inside the wedges $\psi(x)$ vanishes exponentially as $|x| \to \infty$ [2].

However, if $\varepsilon \neq 0$ in equation (1.0.7), the solution of the eigenvalue equation using

WKB has the following form

$$y(x) \sim c_2 Q^{-\frac{1}{4}}(x) \exp\left[\pm \frac{1}{\varepsilon}\int_a^x dt\sqrt{Q(t)}\right] \sim \exp\left[\pm \frac{1}{\varepsilon}\int_a^x dt\sqrt{Q(t)}\right], \tag{4.2.3}$$

with $Q(t) = V(x) = i^{\varepsilon}(x^{2+\varepsilon})$, then

$$\sqrt{i^{\varepsilon}}\int \sqrt{x^{2+\varepsilon}}dx = \sqrt{i^{\varepsilon}}\int x^{1+\frac{\varepsilon}{2}}dx \sim i^{\frac{\varepsilon}{2}}\frac{2}{n+4}x^{2+\frac{\varepsilon}{2}}. \tag{4.2.4}$$

If

$$i = e^{i\frac{\pi}{2}},$$

then the solution looks like this

$$\psi(x) = e^{\pm x^{2+\frac{\varepsilon}{2}}e^{i\pi\frac{\varepsilon}{4}}}. \tag{4.2.5}$$

We use the negative solution of equation (4.2.5) as $|x| \to \infty$ on the real x axis. Notice that when $\varepsilon = 0$ we recover equation (4.2.2). If $x = re^{i\theta}$ as $r \to \infty$. Then, we have

$$(re^{(i\theta)})^{2+\frac{\varepsilon}{2}} = e^{(2i\theta)}r^2(e^{(i\theta)}r)^{\frac{\varepsilon}{2}}$$

$$\Rightarrow r^{2+\frac{\varepsilon}{2}}\exp\left[i\theta\left(2+\frac{\varepsilon}{2}\right)+i\pi\frac{\varepsilon}{4}\right]$$

$$\Rightarrow \psi(r) \sim \exp\left[-\frac{2}{4+\varepsilon}r^{2+\frac{\varepsilon}{2}}\exp i\underbrace{\left[\theta\left(2+\frac{\varepsilon}{2}\right)+\pi\frac{\varepsilon}{4}\right]}_{\text{phase}}\right]. \tag{4.2.6}$$

Equation (4.2.6) is the WKB solution when $\varepsilon \neq 0$, but since $\psi(x)$ has to approach zero as r goes to infinity then, the oscillatory behavior of the phase has to be equal to zero. The anti-Stokes lines are given by the condition that the phase in equation (4.2.6) for $\psi(r)$ be

equal to zero:

$$\theta\left(2+\frac{\varepsilon}{2}\right)+\pi\frac{\varepsilon}{4}=0. \tag{4.2.7}$$

However,

$$\theta\left(2+\frac{\varepsilon}{2}\right)=-\pi\frac{\varepsilon}{4}$$

$$\Rightarrow \theta=-\pi\frac{\varepsilon}{4}\div\left(\frac{4+\varepsilon}{2}\right)$$

$$\Rightarrow \theta=-\frac{2\pi\varepsilon}{4(4+\varepsilon)}$$

$$\Rightarrow \theta_R=-\frac{\pi\varepsilon}{(8+2\varepsilon)}. \tag{4.2.8}$$

The last equation (4.2.8) gives the angular location of the center of the right wedge. Note that if $\varepsilon\to\infty$ then $\theta_R\to\frac{\pi}{2}$. The center of the left wedge is found using symmetry since both wedges are symmetric with respect to the imaginary axis:

$$\theta_L=-\pi+\frac{\pi\varepsilon}{(8+2\varepsilon)}. \tag{4.2.9}$$

The Stokes lines are given by the condition that the exponential of r in the equation (4.2.6) for $\psi(r)$ be equal to $\pm\frac{\pi}{2}$, then we find the opening angle of the wedges as

$$\frac{\Delta\theta}{2}\left(2+\frac{\varepsilon}{2}\right)=\frac{\pi}{2}$$

$$\Rightarrow \Delta\theta=\frac{2\pi}{(4+\varepsilon)}. \tag{4.2.10}$$

4.3 Solution of H in the Complex Plane

We know that the solution of equation (1.0.6) using $\mathcal{H}$ as in equation (1.0.7) has real eigenvalues for $\varepsilon \geq 0$. In order to obtain these eigenvalues, the equation has to be solved along a contour Γ in the complex plane [24]. The contour Γ has to be contained inside the Stokes wedges defined by the Stokes and anti-Stokes lines.

Suppose we have the following Hamiltonian

$$H_* = \Big(p - A(x)\Big)^2 + V(x), \tag{4.3.1}$$

where H_* is a linear operator and $H_* : \mathcal{F} \to \mathcal{F}$. Furthermore, $\mathcal{F}$ is an analytic function such as $\phi = \mathcal{R} \to \mathcal{C}$ and $A(x)$, $V(x)$ are piece-wise analytic functions in $\mathcal{F}$. Where an analytic function is defined as a function which is smooth, that is all of its derivatives are defined and its Taylor series converges to the function. The Hamiltonian H_* has real and discrete eigenvalues if the boundary conditions are defined along a convenient contour Γ in the complex plane[§]. Then, we express H_* with a complex variable z along Γ. A specific example of equation (4.3.1) is given by equation (1.0.7).

The general parametrization is given by

$$x = -\frac{i}{\alpha}(1 + it)^{\alpha}, \qquad t \in (-\infty, \infty), \tag{4.3.2}$$

where $\alpha = \frac{1}{n}$ and the first and second derivatives [10] are given by

$$\frac{d}{dx} = (1 + it)^{1-\alpha}\frac{d}{dt}. \tag{4.3.3}$$

Thus,

$$\left(\frac{d}{dx}\right)^2 = (1 + it)^{2-2\alpha}\left(\frac{d}{dt}\right)^2 + i(1 - \alpha)(1 + it)^{1-2\alpha}\frac{d}{dt}. \tag{4.3.4}$$

[§]See Appendix B.

Therefore, when choosing the contour inside the wedges we will obtain real eigenvalues. Consider

$$z = 2i\sqrt{1+it} \quad t \in \mathbb{R}, \tag{4.3.5}$$

the parametrization (4.3.5) is used in combination with the shooting method[‡‡] to find the numerical approximation of the eigenvalues of equation (1.0.7).

4.4 Hamiltonians

4.4.1 $\mathcal{H} = p^2 + x^2(ix)^\varepsilon$.

Rewriting the Hamiltonian $\mathcal{H}$ of equation (1.0.7) as a differential equation we have

$$-\psi''(x) + x^2(ix)^\varepsilon\psi(x) = E\psi(x). \tag{4.4.1}$$

The solution to the last equation is obtained using the WKB approximation and semi-classical two turning point theory [4]. The result is given by the Born-Sommerfeld equation:

$$\int_{x_-}^{x_+} \sqrt{E - x^2(ix)^\varepsilon}dx = \left(n + \frac{1}{2}\right)\pi, \tag{4.4.2}$$

where n is the number of bounded states associated with classical periodic orbits and x_-, x_+ are the turning points defined as

$$x_- = E^{\frac{1}{\varepsilon+2}}e^{i\pi(\frac{3}{2}-\frac{1}{\varepsilon+2})}, \quad x_+ = E^{\frac{1}{\varepsilon+2}}e^{-i\pi(\frac{1}{2}-\frac{1}{\varepsilon+2})}. \tag{4.4.3}$$

These two turning points are the roots of $E - x^2(ix)^\varepsilon = 0$, we use the roots of unity relation to find them, where the generic solution is given by $re^{(i\theta)} = re^{i(\theta+2\pi k)}$, $k =$

[‡‡]See Section 4.5.

$0, 1, 2, 3, ...,$. The distance between the turning points is defined as the chord length between them, $x_+ - x_- = crd(\theta) = \sqrt{(1-\cos(\theta))^2 + \sin^2(\theta)} = \sqrt{2 - 2\cos(\theta)} = 2\sin(\frac{\theta}{2})$. The integral part of (4.4.2) can be expressed as

$$\int_{x_-}^{x_+} \sqrt{E - x^2(ix)^\varepsilon}dx = \int_{x_-}^{0} \sqrt{E - x^2(ix)^\varepsilon}dx + \int_{0}^{x_+} \sqrt{E - x^2(ix)^\varepsilon}dx, \qquad (4.4.4)$$

since the classical trajectories evolve around the point $x = 0$. On the next step, we change variables substituting $x = sx_-$ on the first integral and $x = sx_+$ on the second integral. Then, we have

$$\int_{x_-}^{x_+} \sqrt{E - x^2(ix)^\varepsilon}dx = \sqrt{E}(x_+ - x_-)\int_0^1 \sqrt{1 - s^3}ds = \left(n + \frac{1}{2}\right)\pi \qquad (4.4.5)$$

$$\Rightarrow 2\sin\left(\frac{\pi}{\varepsilon+2}\right)E^{\frac{1}{\varepsilon+2}+\frac{1}{2}}\int_0^1 \sqrt{1 - s^{\varepsilon+2}} = \left(n + \frac{1}{2}\right)\pi. \qquad (4.4.6)$$

Notice that the generic solution of the integral is given by

$$\int_0^1 \sqrt{1 - x^n}dx = \frac{\sqrt{\pi}\Gamma(1 + \frac{1}{n})}{2\Gamma(\frac{3}{2} + \frac{1}{n})} \quad for \quad Re(n) > 0 \quad and \quad n = 1, 2, 3, ..., \qquad (4.4.7)$$

where $\Gamma(x)$ is the gamma function and $Re(z)$ is the real part of z. Then,

$$2\sin\left(\frac{\pi}{\varepsilon+2}\right)E^{\frac{1}{\varepsilon+2}+\frac{1}{2}}\frac{\sqrt{\pi}\Gamma(1 + \frac{1}{\varepsilon+2})}{2\Gamma(\frac{3}{2} + \frac{1}{\varepsilon+2})} = \left(n + \frac{1}{2}\right)\pi. \qquad (4.4.8)$$

Finally, solving equation (4.4.8) for E we obtain an approximation of the eigenvalues of Figure 1 on page 3.

$$\boxed{E_n \sim \left[\frac{\Gamma(\frac{3}{2}+\frac{1}{\varepsilon+2})\sqrt{\pi}(n+\frac{1}{2})}{\sin(\frac{\pi}{\varepsilon+2})\Gamma(1+\frac{1}{\varepsilon+2})}\right]^{\frac{2\varepsilon+4}{\varepsilon+4}}, \quad n=0,1,2,...,.} \tag{4.4.9}$$

As an example, we calculate the first eigenvalue using equation (4.4.9) with $n=0$ and $\varepsilon=0$, then

$$E_0 \sim \left[\frac{\Gamma(\frac{3}{2}+\frac{1}{2})\sqrt{\pi}(\frac{1}{2})}{\sin(\frac{\pi}{2})\Gamma(1+\frac{1}{2})}\right]^{\frac{4}{4}}$$

$$\Rightarrow E_0 \sim \left[\frac{\Gamma(\frac{3}{2}+\frac{1}{2})\sqrt{\pi}(\frac{1}{2})}{\sin(\frac{\pi}{2})\Gamma(1+\frac{1}{2})}\right]^{1}$$

$$\Rightarrow E_0 \sim \frac{\Gamma(2)\sqrt{\pi}(\frac{1}{2})}{\sin(\frac{\pi}{2})\Gamma(\frac{3}{2})}$$

$$\Rightarrow E_0 \sim \frac{1\sqrt{\pi}(\frac{1}{2})}{1\Gamma(\frac{3}{2})}$$

$$\Rightarrow E_0 \sim \frac{1\sqrt{\pi}(\frac{1}{2})}{1\frac{\sqrt{\pi}}{2}}$$

$$\Rightarrow E_0 \sim 1.$$

4.4.2 $\mathcal{H} = p^2 + ix^3$.

Solving equation (1.0.7) with $\varepsilon = 1$, the following Hamiltonian is obtained:

$$\mathcal{H} = p^2 + ix^3. \tag{4.4.10}$$

Rewriting the last Hamiltonian $\mathcal{H}$ as a differential equation we have

$$-\psi''(x) + x^3(i)\psi(x) = E\psi(x). \tag{4.4.11}$$

According to WKB method the last Hamiltonian has a solution of the form

$$\int_{x_-}^{x_+} \sqrt{E - x^3(i)}dx = \left(n + \frac{1}{2}\right)\pi, \tag{4.4.12}$$

where n is the number of bounded states and $x_\pm$ are the classical turning points [21]. These turning points are the roots of $E + ix^3 = 0$. Therefore, the two turning points are $x_- \equiv x_1 \Rightarrow E^{\frac{1}{3}} e^{i\frac{(\frac{3\pi}{2})}{3}}$ and $x_+ \equiv x_0 \Rightarrow E^{\frac{1}{3}} e^{i\frac{(\frac{\pi}{2})}{3}}$. The distance between the two points is given by the chord then $x_+ - x_- = 2\sin(\frac{\theta}{2}) = 2\sin(\frac{\pi}{6})$. As the classical trajectories develop near the point $x = 0$, the integral (4.4.12) can be re-written as

$$\int_{x_-}^{x_+} \sqrt{E - x^3(i)}dx = \int_{x_-}^{0} \sqrt{E - x^3(i)}dx + \int_{0}^{x_+} \sqrt{E - x^3(i)}dx. \tag{4.4.13}$$

If we substitute $x = sx_-$ on the first integral and $x = sx_+$ on the second integral we obtain

$$\sqrt{E}(x_+ - x_-)\int_0^1 \sqrt{1 - s^3}ds = \left(n + \frac{1}{2}\right)\pi \tag{4.4.14}$$

$$\Rightarrow \sqrt{E}2\left(E^{\frac{1}{3}}\sin\left(\frac{\pi}{6}\right)\right)\int_0^1 \sqrt{1 - s^3}ds = \left(n + \frac{1}{2}\right)\pi \tag{4.4.15}$$

$$\Rightarrow 2E^{\frac{5}{6}}\sin\left(\frac{\pi}{6}\right)\int_0^1 \sqrt{1 - s^3}ds = \left(n + \frac{1}{2}\right)\pi \tag{4.4.16}$$

$$\Rightarrow 2E^{\frac{5}{6}}\sin\left(\frac{\pi}{6}\right)\frac{\sqrt{\pi}\Gamma(\frac{4}{3})}{6\Gamma(\frac{11}{6})} = \left(n + \frac{1}{2}\right)\pi, \tag{4.4.17}$$

where $\Gamma(x)$ is the gamma function. On the last step we solve for E on equation (4.4.17) to get the eigenvalues

$$E_n \sim \left[\frac{6\Gamma(\frac{11}{6})(n+\frac{1}{2})}{\sin(\frac{\pi}{3})\sqrt{\pi}\Gamma(\frac{4}{3})}\right]^{\frac{6}{5}}, \quad n = 0, 1, 2, ..., . \tag{4.4.18}$$

The first eigenvalue at $n = 0$ is

$$E_0 \sim \left[\frac{6\Gamma(\frac{11}{6})(\frac{1}{2})}{\sin(\frac{\pi}{3})\sqrt{\pi}\Gamma(\frac{4}{3})}\right]^{\frac{6}{5}} \tag{4.4.19}$$

$$\Rightarrow E_0 \approx 1.09427. \tag{4.4.20}$$

The result of equation (4.4.20) is shown in Figure 6.

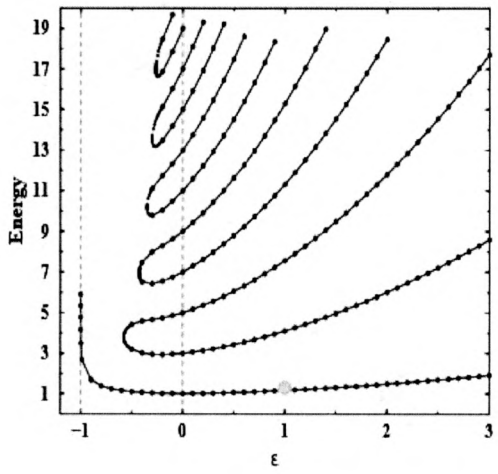

Figure 6: The graph shows the semi-classical approximation of one eigenvalue of $\mathcal{H}$ with $\varepsilon = 1$ and $n = 0$. The y axis shows the values of energy given in units of $\frac{\hbar w}{2}$.

4.4.3 $\mathcal{H} = p^2 + x^4$.

In this section we will show that the Hamiltonian of equation (1.0.7) with $\varepsilon = 2$ has real and positive eigenvalues [7]. Let $\mathcal{H} = p^2 + x^4$ but for the sake of argument we will add the $2m$ constant as well as a γ parameter that belong to the real numbers. Then we have

$$\mathcal{H} = \frac{1}{2m}p^2 - \gamma x^4. \tag{4.4.21}$$

In order to show that the spectrum of equation (4.4.21) is real and positive we will show that it is similar to the spectrum of the following Hermitian Hamiltonian

$$\mathcal{H} = \frac{1}{2m}x^2 + 4\gamma p^4 + \hbar\sqrt{\frac{2\gamma}{m}}p. \tag{4.4.22}$$

As usual we solve equation (1.0.7) using the $\hat{p}$ operator and we obtain the following equation

$$\frac{\hbar^2}{2m}\psi''(x) - \gamma x^4\psi(x) = E\psi(x). \tag{4.4.23}$$

In order to obtain the solution to the last equation we use the following parametrization $x = -2i\sqrt{(1+it)}$, where $t \in (-\infty, \infty)$. Then, we calculate the derivatives following the format of equations (4.3.3) and (4.3.4) then, we replace it back in equation (4.4.23). Also, we have $\psi(x) = \phi(t)$, then

$$\frac{d}{dx} = \sqrt{(1+it)}\frac{d}{dt}, \tag{4.4.24}$$

$$\left(\frac{d}{dx}\right)^2 = (1+it)\left(\frac{d}{dt}\right)^2 + \frac{1}{2}i\frac{d}{dt}, \tag{4.4.25}$$

$$\frac{\hbar^2}{2m}\left[(1+it)\phi''(t) + \frac{1}{2}i\phi'(t)\right] - 16\gamma(1+it)^2\phi(t) = E\phi(t). \tag{4.4.26}$$

In order to obtain the solution of equation (4.4.26) we take a Fourier transform given by

$$f(p) = \int dt\, e^{i\frac{pt}{\hbar}}\phi(t), \tag{4.4.27}$$

where

$$it \to \hbar\frac{d}{dp}, \quad \frac{d}{dt} \to -\frac{ip}{\hbar},$$

therefore, we have

$$-16\gamma\hbar^2 f''(p) + \hbar\left(\frac{p^2}{2m} - 32\gamma\right)f'(p) + \left(\frac{p^2}{2m} + \frac{3\hbar p}{4m} - 16\gamma\right)f(p) = Ef(p). \quad (4.4.28)$$

The next step is to eliminate the term with the first derivative for equation (4.4.28) in order to make it similar to the Schrödinger equation. We introduce a new change of variables $f(p) = Q(p)g(p)$, where $g(p)$ is the new dependent variable. We choose $Q(p)$ to remove the derivative, so the condition imposed on $Q(p)$ is as follows

$$\frac{Q'(p)}{Q(p)} = \frac{p^2}{64m\gamma\hbar} - \frac{1}{\hbar}, \quad (4.4.29)$$

$$\frac{Q''(p)}{Q'(p)} = \frac{p}{32m\gamma\hbar} + \left(\frac{p^2}{64m\gamma\hbar} - \frac{1}{\hbar}\right)^2. \quad (4.4.30)$$

Then using the last condition equation (4.4.28) becomes

$$-16\gamma\hbar^2 g''(p) + \left(\frac{p^4}{256m^2\gamma} + \frac{\hbar p}{4m}\right)g(p) = Eg(p). \quad (4.4.31)$$

On the final step we rescale p as follows $p \to \sqrt{32m\gamma p}$ then, the last equation becomes

$$-\frac{\hbar^2}{2m}g''(p) + \left(4\gamma p^4 + \hbar\sqrt{\frac{2\gamma}{m}}p\right)g(p) = Eg(p). \quad (4.4.32)$$

Therefore, equation (4.4.32) is similar to the Hamiltonian in (4.4.22) but equation (4.4.22) is real and the boundary condition is imposed on the real axis. Thus, the eigenvalues of equation (4.4.22) are real. Then, it follows that the eigenvalues of equation (4.4.21) are real too.

4.5 Eigenvalues of H Numerical

4.5.1 The Shooting Method

In order to find numerically the eigenvalues of equation (1.0.6) with a complex Hamiltonian we use the shooting method to estimate the eigenvalues and then use the Runge-Kutta method to solve the differential equation with an initial value problem. Suppose we have a second order differential equation of the form

$$y'' = f(x, y, y'), \quad for \ a \leq x \leq b, \tag{4.5.1}$$

with the boundary condition on the solution as

$$y(a) = \alpha \ and \ y(b) = \beta, \tag{4.5.2}$$

for some constants α and β this equation has a unique solution if the function f and its partial derivatives are continuous. The partial derivative with respect to y is positive and bounded with respect to y'. In order to make the problem linear we define the function f as follows

$$f(x, y, y') = p(x)y' + q(x)y + r(x). \tag{4.5.3}$$

To approximate the unique solution of the linear boundary problem we will consider two initial value problems such as

$$y'' = p(x)y' + q(x)y + r(x) \ for \ a \leq x \leq b \ where \ y(a) = \alpha \ and \ y'(a) = 0 \tag{4.5.4}$$

and

$$y'' = p(x)y' + q(x)y \ \ for \ \ a \leq x \leq b \ \ where \ \ y(a) = 0 \ \ and \ \ y'(a) = 1. \tag{4.5.5}$$

The last two equations have unique solutions. If $y_1(x)$ is the solution of equation (4.5.4) and $y_2(x)$ is the solution of equation (4.5.5) and $y_2(x) \neq 0$, then

$$y(x) = y_1(x) + \frac{\beta - y_1(b)}{y_2(b)} y_2(x). \tag{4.5.6}$$

Where equation (4.5.6) is the solution of the differential equation (4.5.1) with the initial boundary conditions (4.5.2). This is called the weighted sum [17]. In order to use the shooting method, it is necessary to choose an eigenvalue and a matching point x_m which lies inside the boundaries of the problem such as $a \leq x_m \leq b$. Consider the following equation

$$y'' = (V(x) - E)\psi(x) \quad x \in (a, b), \tag{4.5.7}$$

with the following boundary conditions

$$a_0\psi(a) + b_0\psi'(a) = 0, \tag{4.5.8}$$

$$a_1\psi(b) + b_1\psi'(b) = 0, \tag{4.5.9}$$

where the constants a_0, b_0, a_1, b_1 are not zero at the same time. Then, we transform the problem into two first-order initial value problems, then

$$u_l'(x) = (v(x) - E)\psi_l(x), \qquad \psi_l'(x) = u_l(x), \tag{4.5.10}$$

$$u_r'(x) = (v(x) - E)\psi_r(x), \qquad \psi_r'(x) = u_r(x), \tag{4.5.11}$$

where l stands for left approximation and r stands for right approximation,

$$l(a) = -b_0, \;\; \psi_l'(a) = a_0, \;\; \psi_r(b) = -b_1, \;\; \psi_r'(b) = a_1. \tag{4.5.12}$$

Then, it is necessary to choose an initial estimate for the eigenvalue E and solve the equation for $\psi_l(x)$ on the interval $[a, x_m]$ and $\psi_r(x)$ on the interval $[x_m, b]$. The solutions of these equations are obtained by changing the values of E until they are equal at the matching point. When these two functions are equal, the correct eigenvalue is calculated. Then,

$$\psi_l(x_m) = \psi_r(x_m) \;\; and \;\; \psi_l'(x_m) = \psi_r'(x_m). \tag{4.5.13}$$

Let's consider the following equation

$$-\psi''(x) = (E + (ix)^N)\psi(x), \qquad \lim x \to \pm\infty. \tag{4.5.14}$$

The boundary conditions of the last Schrödinger equation are $(-\infty, +\infty)$. However, we have to pick a definite value L where the boundary conditions are $(-L, L)$. Note that the exponent N is defined as $N = \varepsilon + 2$ then, equation (4.5.14) is a shifted equation (4.1.4). The boundary conditions are as follows $\psi_l(a) = 0, \;\; \psi_l'(a) = 1, \;\; \psi_r(b) = 0, \;\; \psi_r'(b) = 1$ where $a = -L$ and $b = +L$ [30].

Following this method, we use the Matlab to calculate the eigenvalues of equation (4.5.12). The codes $star\_normal.m$ and $ode\_fun.m$ can be found in tables 2 and 3[¶] . The codes are a modification of the program presented by G. Wessel [30]. The running time of the program was approximately 1600 seconds. A Matlab 2016 version was used to

[¶]See Appendix C.

write the codes. The code was run in a Dell computer, model Inspiron $13-7000$ series with a 512 GB solid state drive. The final result in Figure 7 shows the eigenvalues of equation (1.0.7) with a shift by 2 of the original work by Bender (Figure 1 page 3).

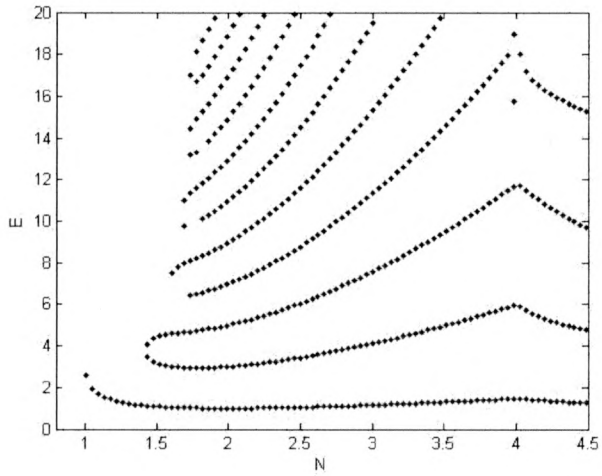

Figure 7: Numerical eigenvalues of equation (1.0.7). The potential in this graph is defined by $V(x) = -(ix)^N$ and we observe E vs N. Notice that $N = \varepsilon + 2$. This is a shifted graph of equation (1.0.7).

The numerical solution in the complex plane of the Schrödinger equation is achieved by using a contour inside the Stokes wedges as explained in section 4.3. Using the contour (4.3.5) but with x instead of t we have $z = 2i\sqrt{1+ix}$, where $x \in \mathbb{R}$. If we apply this contour to equation (4.5.14) then we have the following equations

$$\frac{d^2\psi(z)}{dz^2} = \Big(-E - (iz)^N \Big)\psi(z) \tag{4.5.15}$$

$$\Rightarrow \frac{d^2\psi}{dx^2}\left(\frac{dx}{dz}\right)^2 + \frac{d\psi}{dx}\frac{d^2x}{dz^2} = \Big(-E - (iz)^N \Big)\psi$$

$$\Rightarrow -\frac{d^2\psi}{dx^2}\left(\frac{z^2}{4}\right) + \frac{d\psi}{dx}\frac{i}{2} = \Big(-E - (iz)^N \Big)\psi$$

$$\Rightarrow \frac{d^2\psi}{dx^2} - \left(\frac{2i}{z^2}\right)\frac{d\psi}{dx} = E + (iz)^N \frac{4}{z^2}\psi$$

$$\Rightarrow \frac{d^2\psi}{dx^2} = E + (iz)^N \frac{4}{z^2}\psi + \left(\frac{2i}{z^2}\right)\frac{d\psi}{dx}.$$

Therefore,

$$\psi''(x) = \frac{-E + 2^N(1+ix)^{\frac{N}{2}}}{1+ix}\psi(x) - \frac{i}{2(1+ix)}\psi'(x), \tag{4.5.16}$$

where

$$\frac{z^2}{4} = \frac{(-2i)^2(\sqrt{1+ix})^2}{4}$$

$$z^2 = -4(1+ix).$$

Using equation (4.5.16) we calculate the eigenvalues with Matlab codes, $star\_contour.m$ and $ode\_contour$. These codes can be found on tables 4 and 5. The running time of the program was approximately 2520 seconds and the final result shows the eigenvalues presented in Figure 8.

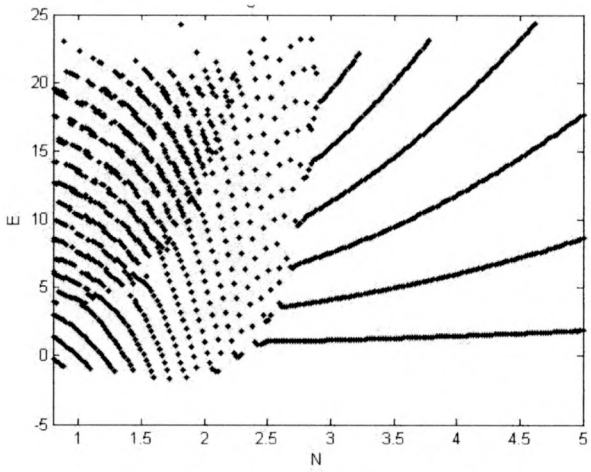

Figure 8: Numerical eigenvalues of the potential $V(x) = -(iz)^N$ where z is a parametrization such as $z = -2i\sqrt{1+ix}$. We observe E vs N.

5 Concluding Remarks

In this thesis we have provided an introduction to Quantum Mechanics for non-Hermitian Hamiltonians with $\mathcal{PT}$ symmetry. We reviewed the literature from the main authors in the field. We established the main axioms of the theory pointing out the similarities and differences with classical Quantum Mechanics. In order to do so, the symmetries $\mathcal{P}$ and $\mathcal{T}$ have been explored in conjunction with a non-Hermitian Hamiltonian. An operator $\mathcal{C}$ has been introduced to define the $\mathcal{CPT}$ inner product. We have shown results using WKB approximation and semi-classical approaches to reconstruct the main equations that the theory uses in order to find a real spectrum. The shooting method, a numerical approximation, was used to confirm the real spectra of the Hamiltonian.

To underline the main features of the theory such as broken and unbroken symmetry, the $\mathcal{C}$ operator and the $\mathcal{CPT}$ inner product examples have been provided for the two-level system. Furthermore, different potentials and their solutions have been presented. In some cases, a parametrization of the potential was needed in order to solve the differential equation described by the Hamiltonian in the complex plane.

Finally, we observe that non-Hermitian Hamiltonian systems with $\mathcal{PT}$ symmetry can be considered as an extension of Quantum Mechanics into the complex plane provided that a positive definitive inner product can be defined. Otherwise, the theory can be reduced to several non-Hermitian Hamiltonian families that possess real eigenvalues under $\mathcal{PT}$ symmetry. Much more theoretical and practical research in the field must be done to get a comprehensive theory of non-Hermitian Quantum Mechanics.

6 Bibliography

[1] Ablowitz, M.J. and Fokas, A.S. (2003) "Complex Variables." Second Edition. Cambridge. Cambridge University Press. Print.

[2] Bender, C.M. "Making sense of non-Hermitian Hamiltonians ." (2007): arXiv. web. 9 March 2007.

[3] Bender, C.M., Berntson, B.K., Parker, D. and Samuel, E. "Observation of PT phase transition in a simple mechanical system." (2012): arXiv. Web. 21 June 2012.

[4] Bender, C.M., Berry, M.V. and Mandilara, A. "Generalized PT symmetry and real spectra." (2002): Journal of Physics A: Mathematical and General. Volume 37, L467L471.

[5] Bender, C.M. and Boettcher, S. "Real spectra in non-Hermitian Hamiltonians Having PT Symmetry." Phys. Rev. Lett. 80, 5243. 1998.

[6] Bender, C.M., Boettcher, S. and Meisinger, P.N. "PT-symmetric quantum mechanics." J. Math. Phys. 40, 2201. 1999.

[7] Bender, C.M., Brody, D.C., Chen, J.H., Jones, H.F., Milton, K.A. and Ogilvie, M.C. "Equivalence of a complex PT-symmetric quartic Hamiltonian and a Hermitian quartic Hamiltonian with an anomaly." Phys. Rev. D 74. 025016.

[8] Bender, C.M., Brody, D.C. and Jones, H.F. "Complex extension of Quantum Mechanics." (2002): Physical Review Letter. Volume 89, Number 27.

[9] Bender, C.M. and Hook, D.W. "Universal spectral behavior of $x^2(ix)^\varepsilon$ potentials." (2012): arXiv. web. 20 May 2012.

[10] Bender, C.M. and Hook, D.W. "Exact isospectral pairs of PT symmetric Hamiltonians." (2008): Journal of Physics A: Mathematical and Theoretical. Volume 41, 244055.

[11] Bender, C.M., Hook, D.W. and Klevansky, C.P. "Negative-energy PT-symmetric Hamiltonians." (2012): arXiv. web. 29 March 2012.

[12] Bender, C.M., Meisinger, P.M. and Qinghai, W. "Finite-Dimensional PT -Symmetric Hamiltonians." (2003): arXiv. web. 29 March 2003.

[13] Bender, C.M. and Orszag, S.A. (1978) "Advanced Mathematical Methods for Scien-

tists and Engineers." New York, New York. Springer. Print.

[14] Intentionally omitted.

[15] Berntson, B. Karl. "PT-symmetric models in classical and Quantum Mechanics." (2012). London.

[16] Chai, Z.M. "Heat Transport in PT-Symmetric Harmonic Chains." (2011). Middletown.

[17] Faires, J.D. and Burden, R. (2003) "Numerical Methods." Third Edition. Belmont, California. Brooks Cole. Print.

[18] Goswami, Amit (2003) "Quantum mechanics." Long Grove, Illinois. Waveland Press, Inc. Print.

[19] Griffiths, David J. (2005) "Introduction to Quantum Mechanics." Upper Saddle River, New Jersey. Pearson Education Inc. Print.

[20] Hesketh, G.D. "PT-symmetric optical lattices." (2010). London.

[21] Moiseyev, N. (2011) "Non-Hermitian Quantum Mechanics." Cambridge. Cambridge University Press. Print.

[22] Mostafazadeh, Ali. "Pseudo-Hermitian representation of Quantum Mechanics." (2011): arXiv. web. 7 February 2011.

[23] Intentionally omitted.

[24] Mostafazadeh, Ali. "Pseudo-Hermitian description of PT-symmetric systems dened on a complex contour." (2005): Journal of Physics A: Mathematical and General. Volume 38, 3213.

[25] Rudin, W. (1976) "Principles of Mathematical Analysis." Third Edition. Singapore. McGraw-Hill Book Company. Print.

[26] Sakurai, J.J. and Napolitano, J. (2011) "Modern Quantum Mechanic." Second Edition. Upper Saddle River, New Jersey. Pearson Education Inc. Print.

[27] Smith, K. "Non-Hermitian Quantum Mechanics." (2010). Cleveland.

[28] Wang, Q. "2×2 PT-symmetric matrices and their applications." (2013): Philosophical Transactions of the Royal Society A.

[29] Weigert, S. "Completeness and orthonormality in pt-symmetric quantum systems." (2003): Physical Review A 68, 062111.

[30] Wessels, G.J.C. "A numerical and analytical investigation into non-Hermitian Hamiltonians." (2008). Matieland.

[31] Zheng, M.C. "Non-Hermitian dynamics: Examples from disordered microwave cavities and classical optics." WesScholar, April 2010.

7 Appendix A

Definition 1. *Time dependent Schrödinger equation:*

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} = -\left[\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(r,t)\right]\psi(r,t), \tag{7.0.1}$$

where $\hbar = \frac{h}{2\pi}$ *is the reduced Planck's constant, where* $h = 6.62607 \times 10^{-34} J \cdot s$ *is the Planck's constant and* m *is the mass of the particle.*

Definition 2. *An operator is an instruction to do something to the function that follow. As an example we have the position operator defined as* $\hat{r} = r$ *and the momentum operator defined as* $\hat{p} = -i\hbar\nabla$.

Definition 3. *The Nabla operator is defined as* $\nabla = \tilde{x}\frac{\partial}{\partial x} + \tilde{y}\frac{\partial}{\partial y} + \tilde{z}\frac{\partial}{\partial z}$.

Definition 4. *We define abstract vector space as a vector space consisting of a set of vectors* $(\overrightarrow{a}, \overrightarrow{b}, \overrightarrow{c}, ...)$ *together with a set of scalars* $(a, b, c, ...)$ *which is closed under two operation vectors: addition and scalar multiplication. Vector addition is commutative and associative, possesses a zero vector and there is an associative inverse vector. Scalar multiplication is distributive and associative.*

Definition 5. *A linear transformation from V to W, where V and W are vector spaces is a function T:* $V \rightarrow$ *W with the following properties;*

$$Additivity\ T(u+v) = Tu + Tv, \tag{7.0.2}$$

for all u *and* $v \in V$.

$$Homogeneity\ T(av) = a(Tv), \tag{7.0.3}$$

for all $a \in F$ *and all* $v \in V$, *where F is the field of rational numbers.*

Definition 6. *Self ad-joint: Let T be a linear transformation on a complex vector space V with inner product. We will say that T is self ad-joint (Hermitian) if $T = T^*$, then it is a linear transformation from V to itself. An $n \times n$ real or complex matrix A is self ad-joint or Hermitian if $A = A^*$. We use the notation $^{(*)}$ to denote a self ad-joint transformation.*

Definition 7. *The Hilbert space is a generalization of the Euclidean space which is a three-dimensional vector space provided with a dot product.*
The dot Product is defined as

$$(x_1, x_2, x_3) \cdot (y_1, y_2, y_3) = x_1 y_1 + x_2 y_2 + x_3 y_3, \tag{7.0.4}$$

where x_i, y_i denote vector space coordinates and $i = 1, 2, 3, ...,$
with the following properties;

- *dot product is symmetric, $x \cdot y = y \cdot x$,*
- *dot product is linear, $(ax_1 + bx_2) \cdot y = ax_1 \cdot y + bx_2 \cdot y$, where a and b are real parameters and x, y are vectors,*
- *dot product is positive definitive, $x \cdot x \geq 0$ where x is a vector.*

We use the notation $(\cdot)$ to denote the dot product.

An operation of two vectors that satisfies the last three conditions is defined as an inner product. A vector space with this inner product condition is defined as an inner product space.

Definition 8. *A unitary operator is an operator which has the following conditions;*

$$U^\dagger U = 1, \tag{7.0.5}$$

$$UU^\dagger = 1. \tag{7.0.6}$$

Definition 9. *A symmetric matrix is defined as a square matrix that is equal to its transpose. Then, a matrix is symmetric if* $A = A^T$.

Definition 10. *An anti-linear transformation from* V *to* W *is a function* $T : V \to W$ *from a complex vector space to another if*

$$T(au + bv) = \hat{a}T(u) + \hat{b}T(v), \tag{7.0.7}$$

where $a, b \in \mathbb{C}$, $u, v \in V$ *and* $\hat{a}, \hat{b}$ *are the complex conjugate of* a, b.

Definition 11. *Square Integrable Function is defined as a function, real or complex, for which the integral of the square of the absolute value is finite. Then,*

$$\int_{-\infty}^{\infty} |f(x)|^2 dx < \infty. \tag{7.0.8}$$

L_2 *denotes the set of integrable functions.*

Definition 12. *Parity operator definitions: The expectation value of* $\boldsymbol{x}$ *taken with respect to the space inverted state has opposite signs. Since,*

$$\langle\alpha|\, \mathcal{P}^\dagger \boldsymbol{x} \mathcal{P}\, |\alpha\rangle = -\langle\alpha|\, \boldsymbol{x}\, |\alpha\rangle\,. \tag{7.0.9}$$

This is accomplished if

$$\mathcal{P}^\dagger \boldsymbol{x} \mathcal{P} = -\boldsymbol{x} \tag{7.0.10}$$

or

$$\boldsymbol{x}\mathcal{P} = -\mathcal{P}\boldsymbol{x}, \tag{7.0.11}$$

where it has been used that $\mathcal{P}$ *is unitary. Therefore,* $\boldsymbol{x}$ *and* $\mathcal{P}$ *must anti-commute, where the anti-commute condition is given when the swapping of any two arguments negates the result.*

Furthermore, we discuss the eigenket of the position operator under parity, claiming that

$$\mathcal{P}\left|\boldsymbol{x}'\right\rangle = e^{i\theta}\left|-\boldsymbol{x}'\right\rangle, \tag{7.0.12}$$

where $e^{i\theta}$ is a phase factor, $\theta \in \mathcal{R}$. To prove this assertion note that

$$\boldsymbol{x}\mathcal{P}\left|\boldsymbol{x}'\right\rangle = -\mathcal{P}\boldsymbol{x}\left|\boldsymbol{x}'\right\rangle = -(\boldsymbol{x}')\mathcal{P}\left|\boldsymbol{x}'\right\rangle. \tag{7.0.13}$$

The last equation states that $\mathcal{P}\left|\boldsymbol{x}'\right\rangle$ is an eigenket of $\boldsymbol{x}$ with eigenvalue $-\boldsymbol{x}'$ so it must be the same as the position eigenket $\left|\text{-}\boldsymbol{x}'\right\rangle$ up to phase factor.

Taken $e^{i\theta} = 1$ by convention and replacing this in the eigenket equation we have $\mathcal{P}^2\left|\boldsymbol{x}'\right\rangle = \left|\boldsymbol{x}'\right\rangle$; hence

$$\mathcal{P}^2 = 1. \tag{7.0.14}$$

which means that we come back to the same state by applying $\mathcal{P}$ twice. We observe that $\mathcal{P}$ is not only unitary but also Hermitian:

$$\mathcal{P}^{-1} = \mathcal{P}^{\dagger} = \mathcal{P}. \tag{7.0.15}$$

Definition 13. *A left eigenvector is defined as a row vector X_l which satisfies the following condition, $X_l A = \lambda_l X_l$.*

8 Appendix B

Proof of $\mathcal{H}^{\dagger} \neq \mathcal{H}$. We want to prove that the Hamiltonian $\mathcal{H}$ is not Hermitian.

Given: Property of Hermitian operators.

$$\langle f|\hat{Q}f\rangle = \langle \hat{Q}f|f\rangle \quad for\ all\ f(x). \tag{8.0.1}$$

Begin proof: if we replace f by the wave function Ψ we observe the following

$$\langle \Psi|\hat{Q}\Psi\rangle = \int \Psi^{*}\hat{Q}\Psi dx, \tag{8.0.2}$$

where the symbol $(*)$ denotes the complex conjugate of Ψ.

$$\int \Psi^{*}\hat{Q}\Psi dx = \int (\hat{Q}\Psi)^{*}\hat{Q}\Psi dx. \tag{8.0.3}$$

If we replace the operator $\hat{Q}$ by $\mathcal{H}$ we observe that

$$\int \Psi^{*}\mathcal{H}\Psi dx \neq \int (\mathcal{H}\Psi)^{*}\Psi dx \tag{8.0.4}$$

$$\Rightarrow \int \Psi^{*}[p^2 + x^2(ix)^{\varepsilon}]\Psi dx \neq \int ([p^2 + x^2(ix)^{\varepsilon}]\Psi)^{*}\Psi dx$$

$$\Rightarrow \int \Psi^{*}[p^2 + x^2(ix)^{\varepsilon}]\Psi dx \neq \int [p^2 + x^2(-ix)^{\varepsilon}]\Psi^{*}\Psi dx$$

$$\Rightarrow (i)^{\varepsilon} \int \Psi^{*}(p^2 + x^2(x)^{\varepsilon})\Psi dx \neq (-i)^{\varepsilon} \int (p^2 + x^2(x)^{\varepsilon})\Psi^{*}\Psi dx. \tag{8.0.5}$$

Therefore, $\mathcal{H}$ is not Hermitian.

□

- Exact Calculation of eigenvalues of matrix H_a.

$$Det(H_a - \lambda I) = 0, \tag{8.0.6}$$

where λ is the eigenvalue and I is the identity matrix.

Then, $[(v_0 + i\gamma) - \lambda] * [(v_0 - i\gamma) - \lambda] - k^2 = 0$

$\Rightarrow (v_0 + i\gamma) * (v_0 - i\gamma) - (v_0 + i\gamma)\lambda - \lambda(v_0 - i\gamma) + \lambda^2 - k^2 = 0$

$\Rightarrow v_0^2 - v_0 i\gamma + v_0 i\gamma - i^2\gamma^2 - \lambda v_0 - \lambda i\gamma - \lambda v_0 + \lambda i\gamma + \lambda^2 - k^2 = 0$

$\Rightarrow v_0^2 + \gamma^2 - 2\lambda v_0 + \lambda^2 - k^2 = 0$

$\Rightarrow \lambda^2 - 2\lambda v_0 + v_0^2 + \gamma^2 - k^2 = 0.$

Then, solving the last equation for λ we have

$$\lambda = \frac{2v_0 \pm \sqrt{4v_0^2 - 4(1)(v_0^2 + \gamma^2 - k^2)}}{2}$$

$$\Rightarrow \lambda = \frac{2v_0 \pm \sqrt{4v_0^2 - 4v_0^2 - 4\gamma^2 + 4k^2}}{2}$$

$$\Rightarrow \lambda = \frac{2v_0 \pm 2\sqrt{k^2 - \gamma^2}}{2}$$

$$\Rightarrow \lambda = v_0 \pm \sqrt{k^2 - \gamma^2}.$$

Therefore, the eigenvalues of H_a are given by $\lambda = v_0 \pm \sqrt{k^2 - \gamma^2}$.

- Exact Calculation of eigenvalues of matrix H_b.

$$Det(A - \lambda I) = 0, \tag{8.0.7}$$

where A is a square matrix, λ is the eigenvalue and I is the identity matrix. Then, using $A = H_b$ in equation (8.0.7) we have the following $Det(H_b - \lambda I) = 0$ or

$$Det \begin{pmatrix} re^{+(i\theta)} - \lambda & k \\ k & re^{-(i\theta)} - \lambda \end{pmatrix} = 0.$$

Using the Euler formula the last determinant becomes

$$Det \begin{pmatrix} (r\cos(\theta) + ir\sin(\theta)) - \lambda & k \\ k & (r\cos(\theta) - ir\sin(\theta)) - \lambda \end{pmatrix} = 0.$$

Then, $[(r\cos(\theta) + ir\sin(\theta)) - \lambda * (r\cos(\theta) - ir\sin(\theta)) - \lambda] - k^2 = 0$

$\Rightarrow r^2\cos^2(\theta) - r\cos(\theta)ir\sin(\theta) - \lambda r\cos(\theta) + r\cos(\theta)ir\sin(\theta) + r^2\sin^2(\theta) - \lambda ir\sin(\theta) - \lambda r\cos(\theta) + \lambda ir\sin(\theta) + \lambda^2 - k^2 = 0$

$\Rightarrow \lambda^2 - 2\lambda r\cos(\theta) + r^2\cos^2(\theta) + r^2\sin^2(\theta) - k^2 = 0$

$\Rightarrow \lambda^2 - 2\lambda r\cos(\theta) + r^2(\cos^2(\theta) + \sin^2(\theta)) - k^2 = 0.$

The characteristic polynomial is given by

$\lambda^2 - 2\lambda r\cos(\theta) + r^2 - k^2 = 0,$

since

$$\cos^2(\theta) + \sin^2(\theta) = 1, \tag{8.0.8}$$

where the solution of the quadratic equation is as follows

$$\lambda = \frac{2r\cos(\theta)}{2} \pm \frac{\sqrt{4r^2\cos^2(\theta) - 4(1)(r^2 - k^2)}}{2}$$

$$\Rightarrow \lambda = r\cos(\theta) \pm \frac{\sqrt{4r^2\cos^2(\theta) - 4r^2 + 4k^2}}{2}$$

$$\Rightarrow \lambda = r\cos(\theta) \pm \frac{\sqrt{4(r^2\cos^2(\theta) - r^2 + k^2)}}{2}$$

$$\Rightarrow \lambda = r\cos(\theta) \pm \sqrt{(r^2\cos^2(\theta) - r^2 + k^2)}$$

$$\Rightarrow \lambda = r\cos(\theta) \pm \sqrt{(r^2(\cos^2(\theta) - 1) + k^2)}$$

$$\Rightarrow \lambda = r\cos(\theta) \pm \sqrt{k^2 - r^2\sin^2(\theta)}.$$

Therefore, the eigenvalues of the two-level system are given by

$$\epsilon_{\pm} = r\cos(\theta) \pm \sqrt{k^2 - r^2\sin^2(\theta)}. \tag{8.0.9}$$

- We will show that the Hamiltonian H_* and the contour Γ are $\mathcal{PT}$ symmetric if H' is $\mathcal{PT}$ symmetric. In order to find the eigenvalues of equation (4.3.1) we replace x for the complex parameter z as follows

$$\left[-\left(\frac{d}{dz} - iA(z)\right)^2 + V(z)\right]\psi(z) = E_n\psi_n(z), \qquad \psi_n(z) \to 0. \tag{8.0.10}$$

The contour Γ is not unique but it has to stay inside the Stokes wedges as the real part of the contour Γ tends to infinity. Most of the time, the contour Γ is a smooth curve parameterized with a real variable a. There exists a continuous piece-wise function which is differentiable such as; $\xi : \mathbb{R} \to \mathbb{C}$ and $\Gamma = \{(\xi(a)|a \in \mathbb{R}\}$. Now, we define the boundary condition of equation (8.0.10) as

$$lim|\psi_n(\xi(a))| \to 0 \; as \; a \to \pm\infty. \tag{8.0.11}$$

Then, we choose the contour $z = x + iy$ defined in a coordinate system $\mathbb{R}^2 = \mathbb{C}$, which is a smooth and increasing function of x. We define the differentiable function ξ as $\xi(x) = x + if(x)$ where $f : \mathbb{R} \to \mathbb{R}$, then if $z = \xi(x)$ we have that $z = x + if(x)$ and performing the change of variable we obtain

$$\left[-g(x)^2\left(\frac{d}{dx} - ia(x)\right)^2 + ig(x)^3\left(\frac{d}{dx^2}f(x)\right)\left(\frac{d}{dx} - ia(x)\right) + V(x)\right]\psi_n(x) = E_n\psi_n(x), \tag{8.0.12}$$

where $g(x) = \xi'(x)^{-1} = \left(1 + i\frac{d}{dx}f(x)\right)^{-1}$,

$a(x) = g(x)^{-1}A(x + if(x))$,

$v(x) = V(x + if(x))$,

$\psi_n(x) = \psi_n(x + if(x))$.

The boundary condition of equation (8.0.12) becomes $\psi(x) \to 0 \; as \; x \to \pm\infty$ where the domain $\in L_2(\mathbb{R})$. Then, the eigenvalue problem of equation (4.3.1) is similar to the eigenvalue problem of the following equation

$$H' = g(x)^2(p - a(x))^2 - g(x)^3(p - a(x))\frac{d}{dx^2}f(x) + v(x). \tag{8.0.13}$$

If we apply the condition of $\mathcal{PT}$ symmetric system to the Hamiltonian H' then we have

$$\mathcal{PT}H'\mathcal{PT} = (g(-x)^*)^2(p - a(-x)^*)^2 - (g(-x)^*)^3(p - a(-x)^*)\frac{d}{dx^2}f(-x)^* + v(-x)^*. \tag{8.0.14}$$

In order for H' to be $\mathcal{PT}$ symmetric the following conditions must hold

$$(g(-x)^*)^2 = g(x)^2, \tag{8.0.15}$$

$$g(-x)^* f(-x)^* = g(-x)^* \frac{d}{dx^2} f(x), \tag{8.0.16}$$

$$a(-x)^* = a(x), \quad v(-x)^* = v(x). \tag{8.0.17}$$

It follows since f is real and x can be 0, then $f(x)^* = -f(x)$,

$$A(u)^*|_{u=-(x+if(x))} = A(x + if(x)), \tag{8.0.18}$$

$$V(u)^*|_{u=-(x+if(x))} = V(x + if(x)). \tag{8.0.19}$$

Therefore, the conditions (8.0.15-17) implies that $z(x)^* = z(x)$ and (8.0.18-19) shows that A and V are both $\mathcal{PT}$ symmetric. Therefore, the Hamiltonian H_* and the contour Γ are $\mathcal{PT}$ symmetric if H' is $\mathcal{PT}$ symmetric [30].

9 Appendix C

9.1 Matlab Programs

Table 2: star_normal.m

```
clear
close all
clc

% Accuracy Settings
abstol  = 1e-3;
reltol  = 1e-3;
zerotol = 1e-3;

% Grid Size
g1 = 100;
g2 = 12;
n1 = linspace(0.8,5,g1);
n2 = linspace(0,20,g2);

% Initializaion
E = NaN(length(n1)*length(n2),2);
k = 1;
tstart = tic;

% Loop through all grid points: (E,N) pairs
for i = n1,
    for j = n2,
        tic;
        f = fzero('ode_fun',j,zerotol,i,abstol,reltol); tt =
            toc;
        fprintf('k = %4d/%3d   N = %2.4e   Et = %2.4e   E =
           %2.4e   Elapsed time = %2.4f sec\n',k,length(n1)*
           length(n2),i,j,f,tt);
        E(k,:) = [i f];
        k = k + 1;
    end
end
tt = toc(tstart); fprintf('\n\nTotal Elapsed Time: %4.4f sec
   \n',tt);

% Plot Results
plot(E(:,1),E(:,2),'b.','markersize',8); axis([0.8 4.5 0
   20]);
title('Eigenvalues of V(x) = -(ix)^N'); xlabel('N'); ylabel(
   'E');
```

Table 3: ode_fun.m

```
function phi = ode_fun(E,N,abstol,reltol)

% Initial Conditions
xm = 0;
a  = -10;
b  = 10;
y0 = 0;
v0 = 1;

% Integration Settings
options = odeset('Abstol',abstol,'RelTol',reltol);

% Shrdinger-function with PT symmetric potential
F = @(x,w) [w(2); (-(1i*x)^N - E)*w(1)];

% RK4 algorithm
[~,WL] = ode45(F,[a xm],[y0 v0],options);
YL = WL(:,1); VL = WL(:,2);
YL = YL/max(abs(YL)); VL = VL/max(abs(VL));

[~,WR] = ode45(F,[b xm],[y0 v0],options);
YR = WR(:,1); VR = WR(:,2);
YR = YR/max(abs(YR)); VR = VR/max(abs(VR));

% Solution (phi)
phi = VR(end)*YL(end) - VL(end)*YR(end);
phi = real(phi);

end
```

Table 4: star_contour.m

```
clear
close all
clc

% Accuracy Settings
abstol  = 1e-3;
reltol  = 1e-3;
zerotol = 1e-3;

% Grid Size
g1 = 200;
g2 = 15;
n1 = linspace(0.8,5,g1);
n2 = linspace(0,20,g2);

% Initializaion
E = NaN(length(n1)*length(n2),2);
k = 1;
tstart = tic;

% Loop through all grid points: (E,N) pairs
for i = n1,
    for j = n2,
        tic;
        f = fzero('ode_contour',j,zerotol,i,abstol,reltol);
            tt = toc;
        fprintf('k = %4d/%3d   N = %2.4e   Et = %2.4e   E =
            %2.4e   Elapsed time = %2.4f sec\n',k,length(n1)*
            length(n2),i,j,f,tt);
        E(k,:) = [i f];
        k = k + 1;
    end
end
tt = toc(tstart); fprintf('\n\nTotal Elapsed Time: %4.4f sec
    \n',tt);

% Plot Results
plot(E(:,1),E(:,2),'b.','markersize',5); axis([0.8 5 -5 25])
    ;
title('Shooting Method: $$z = -2i \sqrt{1 + ix}$$','
    interpreter','latex');
xlabel('N'); ylabel('E');
```

Table 5: ode_contour.m

```
function phi = ode_contour(E,N,abstol,reltol)

% Initial Conditions
xm = 0;
a  = -10;
b  = 10;
y0 = 0;
v0 = 1;

% Integration Settings
options = odeset('Abstol',abstol,'RelTol',reltol);

% Contour function
contour = @(t,y,tE,tN) ...
    [y(2);
    (- 2^tN*(1 + 1i*t)^(tN/2) - tE)*y(1)/(1 + 1i*t) - (1i/2)
       *y(2)/(1 + 1i*t)];

% RK4 algorithm
[~,WL] = ode45(@(t,y) contour(t,y,E,N),[a xm],[y0 v0],
   options);
YL = WL(:,1); VL = WL(:,2);
YL = YL/max(abs(YL)); VL = VL/max(abs(VL));

[~,WR] = ode45(@(t,y) contour(t,y,E,N),[b xm],[y0 v0],
   options);
YR = WR(:,1); VR = WR(:,2);
YR = YR/max(abs(YR)); VR = VR/max(abs(VR));

% Solution (phi)
phi = VR(end)*YL(end) - VL(end)*YR(end);
phi = real(phi);

end
```